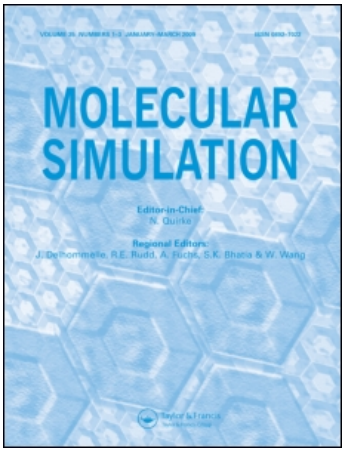

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Spin polarization in GaAs/$Al_{0.24}Ga_{0.76}As$ heterostructures

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Spin polarization in GaAs/$Al_{0.24}Ga_{0.76}As$ heterostructures

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The spontaneous spin polarization of a quantum point contact (QPC) formed by the lateral confinement of a high-mobility two-dimensional electron gas in a GaAs/AlGaAs split gate heterostructure is investigated. Self consistent calculations of the electronic structure of the QPC are performed using the spin-polarized density functional formalism of Kohn and Sham. Spin polarization occurs at low electron densities and exchange interaction is found to be the dominant mechanism driving the local spin polarization within the QPC. The cascading scattering matrix approach is utilized to compute the conductance and a conductance anomaly at ~ 0.5 ($2e^2/h$) has been observed. In addition to this, the sheet density dependence of the 0.7 conduction anomaly is investigated.

Keywords: QPC; 0.7 structure; LDA; 2DEG

1. Introduction

Spintronics, a new branch of electronics, involves the active control and manipulation of spin degrees of freedom in solid-state devices. Spin transport differs from charge transport, as spin is a non-conserved quantity in solids due to spin-orbit and hyperfine coupling. With rapid scaling of CMOS technology the physical gate lengths of transistors have reached atomic length scales where short channel effects the degrade of the device performance drastically. The alternative technologies, like spintronics, can complement the existing scaled CMOS technology to extend Moore's law even further to dimensions as small as 8 nm. Extensive research has been going on in this field to overcome a variety of challenges posed in the form of efficient injection, transport and detection of spin polarized carriers.

Various conductance measurements have been performed on quantum point contacts (QPC) formed by the lateral confinement of a high mobility two-dimensional electron gas (2DEG) in split gate GaAs/AlGaAs heterostructures. Conductance quantization [1] is observed in these mesoscopic devices, and in addition to the integer multiples of $2e^2/h$, some experimental groups have observed an extra feature at $G \sim 0.7$ ($2e^2/h$) [2,3]. This feature at $0.7\,G_o$ has been referred to as "0.7 conduction anomaly" or simply "0.7 structure". This feature has also been shown to vary between ~ 0.5 and 0.7 depending on various parameters like the surface gate geometry, length of the channel and the electron density [4].

The above experimental observations initiated a number of theoretical efforts to understand and explain the 0.7 anomaly [5,6,7]. The most accepted idea is to associate this anomaly with the electron–electron interaction inducing an onset of spontaneous spin polarization in the QPC. Many modeling attempts carried out along these lines have considered simple analytical model potentials to include the spin density functional formalism of Kohn and Sham in the local density approximation (LDA) [7]. The local exchange potential induces spontaneous local magnetization and a spin splitting of the sub-bands. The exchange interaction is, hence, seen to be the dominant mechanism towards the spin splitting.

In this paper, we try to extend the same modeling approach to real potentials obtained from a self consistent 3D Poisson-1D Schrödinger solver. The LDA approximation in the Kohn Sham density functional formalism is used to calculate the total effective potentials for the spin species. The device modeled is a GaAs/$Al_{0.24}Ga_{0.76}As$ modulation doped heterostructure having a 35 nm GaAs quantum well. A schematic view of the device structure simulated in this work is shown in figure 1 where N_{d1} and N_{d2} are the two delta doped layers.

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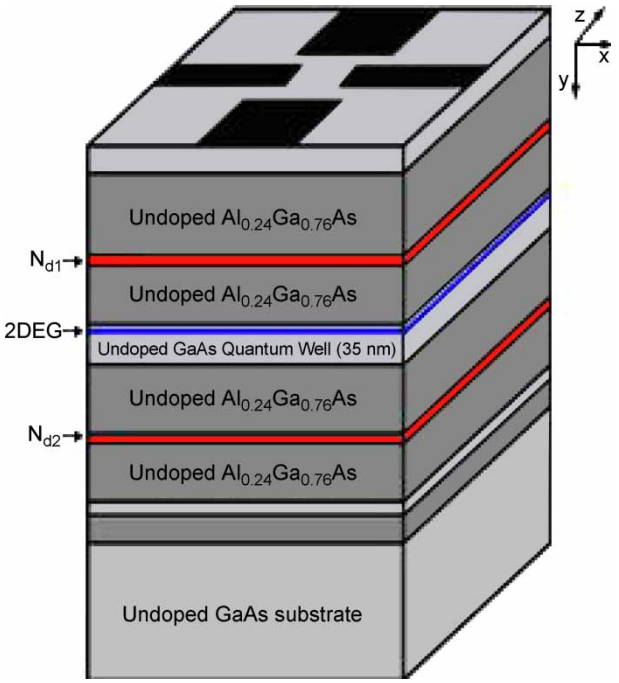

Figure 1. Simulated GaAs/$Al_{0.24}Ga_{0.76}As$ heterostructure with the split gates on top.

2. Theoretical modeling

The simulation procedure, used to obtain the self consistent potential, is comprised of two parts. The first part involves the calculation of the self consistent Hartree potential by using the in-house 3D Poisson-1D Schrödinger solver. The confinement in the growth direction (y direction) is found to be much stronger than the confinement in the z direction and we can assume, with no approximations involved, that only the first sub-band related to the y direction is occupied for low sheet electron densities. We then place the 2DEG in a single plane located at the (as calculated) average distance within the quantum well.

In the next part, the 2D Hartree potential is used in solving the 1D Schrödinger equation in slices along the z direction to capture the confinement at the QPC due to the application of a negative potential on the split gates. The exchange and correlation potential are also included in the one electron Schrödinger equation, which can be expressed as

$$-\frac{\hbar^2}{2m^*}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}\right]\psi^\sigma(x,z)+V_{\text{eff}}(x,z)\psi^\sigma(x,z) = E\psi^\sigma(x,z) \quad (1)$$

via the effective potential term, where

$$V_{\text{eff}}(x,z) = V_{\text{H}}(x,z)+V^\sigma_{\text{exch}}(z)+V^\sigma_{\text{corr}}(z)+g\mu_B B\sigma \quad (2)$$

In equation (2), V_{eff} is the total effective potential, V_{H} is the Hartree potential, V_{exch} and V_{corr} being the exchange and correlation potential where $\sigma = \pm 1/2$. The last term in equation (2), called the Zeeman term, is used as a fictitious potential ($g\mu_B B\sigma = 10^{-6}\,eV$) to trigger the onset of the spin polarization and can be switched off after a few iteration steps.

The exchange potential for a 2DEG, in the LDA is given by [9],

$$V^\sigma_{\text{exch}}(z) = -\frac{e^2}{\varepsilon_0\varepsilon\pi^{3/2}}[n^\sigma(z)]^{1/2} \quad (3)$$

$$n^\sigma(z) = \frac{1}{\pi}\sum_{E^\sigma\le E_F}\left[\frac{2m^*}{\hbar^2}(E_F-E^\sigma)\right]^{1/2}|\psi^\sigma(z)|^2 \quad (4)$$

In equations (3) and (4) E_F is the Fermi energy and n^σ is the electron distribution for all occupied states with spin σ. For the correlation potential, the parametrized form of Tanatar and Ceperley [10] for fully polarized and non-polarized 2DEG's, is adopted. In our calculation we assume $m* = 0.067m_o$ and $g = 0.44$ (representative of bulk GaAs). The reconstructed quantum mechanical 3D density is then used to update the Hartree potential and this procedure is continued until self-consistency (error tolerance of the potential $<5\times10^{-4}$ eV) is reached. The spin polarization of the system is obtained as the difference between the densities of $\uparrow$ and $\downarrow$ electrons:

$$p(x,z) = n^\uparrow(x,z)-n^\downarrow(x,z) \quad (5)$$

The transport phenomena in this structure are investigated using the Landauer-Büttiker formalism. The conductance G of the system is obtained from a multi-channel case of the Landauer formula [11],

$$G = \frac{2e^2}{h}\sum_{m,n}\frac{\nu_n}{\nu_m}|t_{nm}|^2 \quad (6)$$

where t_{nm} is the transmission probability from the mth channel with velocity ν_m to the nth channel with velocity ν_n. The transfer matrix technique for calculation of the transmission coefficient is generally unstable and to stabilize it we use the iteration technique proposed by Usuki *et al.* [12].

3. Simulation results

The important parameters required for the self consistent calculation of the total effective potential—Schottky barrier potential and donor ionization energy—are validated with experimental data by performing the simulations on a Hall bar structure. The simulated sheet densities are in good accordance with the experiment data and fall within the 7% error margins of the experiment. Figure 2 shows the spin splitting obtained when a negative gate voltage of 4 V is applied on the split gates.

The figure shows the energy of the 2 spin electrons along with the Hartree potential as we move along the z direction, i.e. perpendicular to the channel. We see a

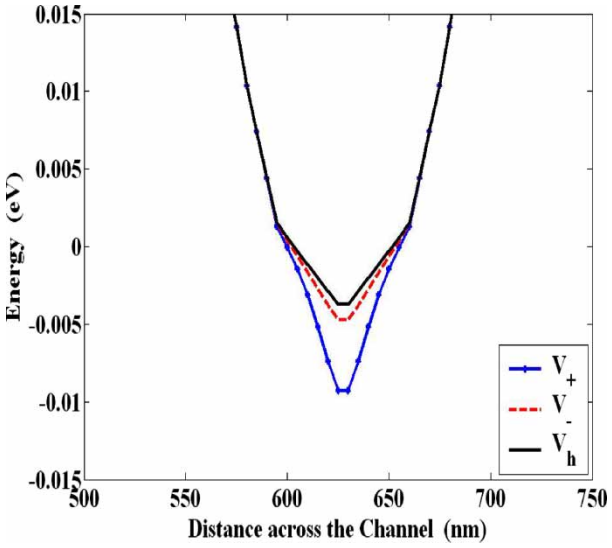

Figure 2. Spin splitting in the total effective potential for the up and down spin electrons for a gate voltage of −4 V.

difference in the effective potentials of the up and down spin electrons as the exchange potential drives one spin towards more negative values than the other spin carriers.

The spontaneous spin polarization in the QPC, given by $p(x, z)$, with −4 V on the split gates is shown in figure 3. This shows the difference in the densities of the two spin species corresponding to a spin splitting of around 2–4 meV.

The conductance–gate voltage characteristics is shown in figure 4. This data shows that there is full spin polarization as one spin goes through the channel and the other spin is reflected. In addition to the plateaus at the integer multiples of $2e^2/h$, there is a point of inflection around 0.5 ($2e^2/h$).

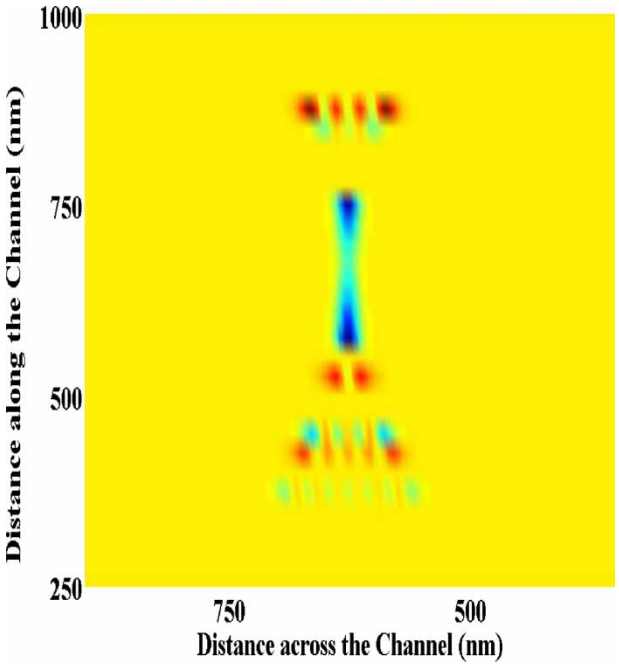

Figure 3. Spontaneous spin polarization observed in the QPC along the *XZ* plane at a split gate voltage of −4 V.

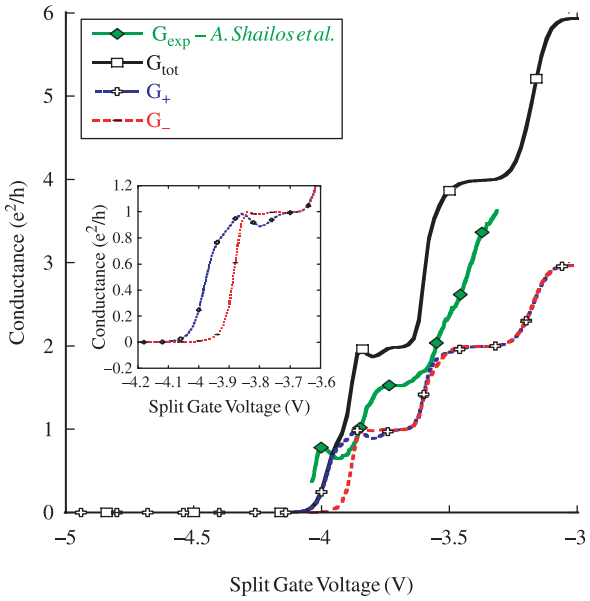

Figure 4. Conductance as a variation of the split gate voltage, Inset shows the full spin polarization of the up and down spin electrons around −4 V.

This result is in agreement with other modeling attempts trying to explain the 0.7 anomaly and is able to explain some of the features observed in experiments [13].

The same type of simulations was carried out for device structures with different sheet densities in an effort to try, to capture the density dependence of the 0.7 structure. This can be done in two ways—by applying a negative bias on the smaller finger gates or by changing the doping in the delta doped layers. This work utilizes the second method to reduce the 2DEG sheet densities. Figure 5 shows the same density dependence of the 0.7 structure for three different sheet densities. There is a feature around *0.5* ($2e^2/h$) for the

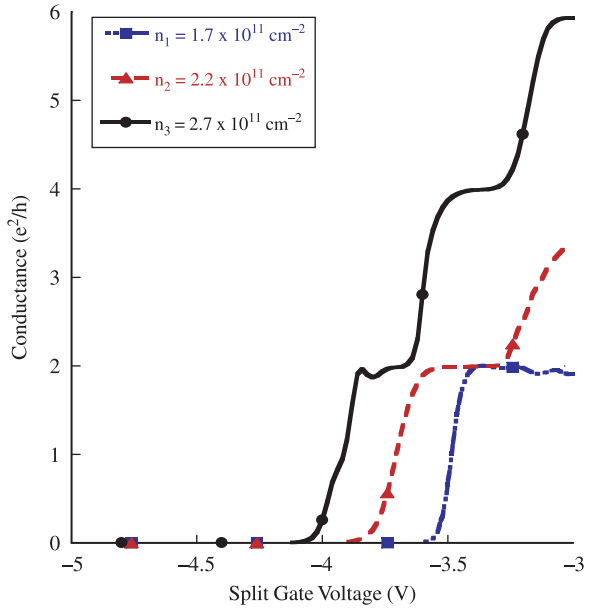

Figure 5. Sheet density dependence of the 0.7 conduction anomaly.

highest n_{2D} case but the transition to 0.7 ($2e^2/h$) is not seen. The transition from 0.7 to 0.5 ($2e^2/h$) has been observed by several experimental groups [14,4] but for much lesser sheet densities, in the order of $10^{10}\,\mathrm{cm}^{-2}$.

4. Conclusions

In summary, we have found evidence of spontaneous spin polarization in realistic QPC devices by developing a self-consistent simulation scheme using Kohn–Sham spin density functional formalism. The exchange interaction is the dominant driver behind the onset of spontaneous spin polarization in the QPC. The density dependence of the 0.7 anomaly was also investigated and although the *0.5* ($2e^2/h$) point of inflection is seen at higher densities, lower electron densities must be included in order to observe the transition to *0.7* ($2e^2/h$). In a future effort, we would like to build a Monte Carlo based transport kernel incorporating all the spin-flip scattering mechanisms to calculate the exact conductance through the QPC.

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