Theoretical Evidence of Spontaneous Spin Polarization in GaAs/AlGaAs Split-Gate Heterostructures

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ABSTRACT

Spintronics is a new branch of electronics which utilizes the spin degree of freedom of an electron rather than the charge, as used in conventional devices. This paradigm by itself provides a huge potential in, for example, high density memories, non volatile reprogrammable logic, quantum computing and various other applications. Extensive research has been going on in the spintronic field to overcome variety of challenges posed in the form of efficient injection, transport and detection of spin polarized carriers from one material to another, etc. To validate the spin splitting in device heterostructures, various conductance measurements have been performed on quantum point contacts (QPC) formed by a lateral confinement of a high mobility two-dimensional electron gas in a modulation doped GaAs/$Al_xGa_{1-x}As$ heterostructure. It has been found that these structures exhibit additional plateaus (below the first plateau) at 0.7 and 0.25 ($2e^2/h$). It this work, the spin-polarized density functional theory of Kohn and Sham is used to calculate the spin dependent features of the quantum point contacts and confirm the recent experimental findings within our group.

The simulation procedure to accomplish this task consists of the following steps. First, the in-house 3D Poisson-1D Schrödinger solver is used to obtain the self consistent Hartree potential and the sheet densities of the two-dimensional electron gas (2DEG) in the GaAs quantum well. For that purpose, the Schrödinger equation is solved in slices along the growth direction. The method has been quite accurate in defining self-consistent potentials in a variety of closed and open GaAs/AlGaAs quantum dots. Then, we make the assumption that the 2DEG is located at the average distance within the quantum well which means that the 2D Hartree potential is an accurate representation of the full 3D system. The potential profile of the 2DEG is next used to calculate the total effective potential[1] for the up spin and the down spin electrons. The total potential is obtained by adding the exchange[2] and correlation[3] energies to the Hartree potential. The resultant 2D potential is then used in a 1D Schrödinger equation solver that calculates the eigenstates along the z-direction (perpendicular to the channel) to get the 1D electron density and, thereby, the sheet densities for the up and down spin states separately. This method is repeated iteratively until self consistency in the total potential is achieved.

The simulation results that utilize the above-described scheme are shown in Figures 2–5. Figure 2 shows the gate voltage dependence of the simulated sheet density and the corresponding experimental data. The simulated heterostructure exhibits pinch-off around -5 V on the split gates (Figure 3). We see an appreciable spin splitting between the up and down spin electrons at Vg = - 4.0 V (Fig. 4). We also see spontaneous spin polarization and the presence of resonance states in Fig. 5. The conductance calculations for this device structure are currently being pursued and the results from these investigations will be presented at the conference.

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[3] B. Tanatar and D.M. Ceperley, Phys. Rev. B **39**, 5005 (1989).

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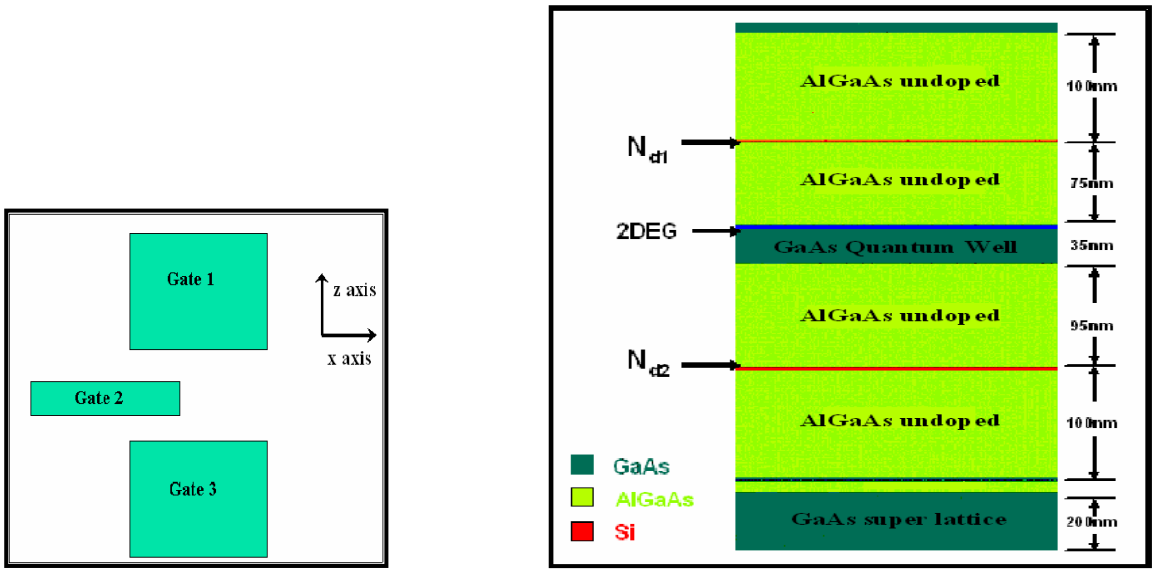

Figure 1: Schematic description of the MBE grown GaAs/$Al_{0.24}Ga_{0.76}As$ heterostructure being simulated. The figure on the left shows the split gates (Gate 1 and 3) and the finger gate (Gate 2). The hetero-structure, having a 35 nm GaAs quantum well and delta doped regions (doped to 10^{12} /cm^2 of Si) is shown on the right panel.

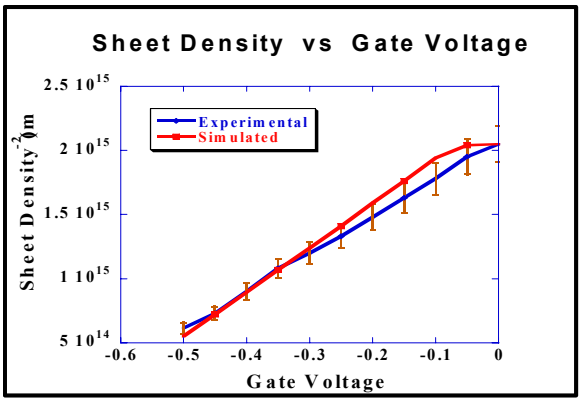

Figure 2: Variation of the sheet density in the quantum well.

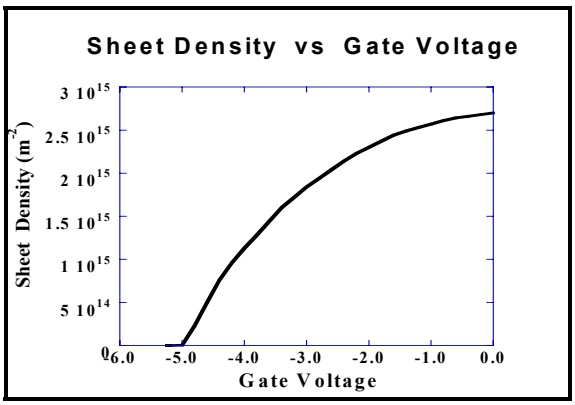

Figure 3: Variation of the sheet density with gate voltage (split gates) and finger gate at 0V.

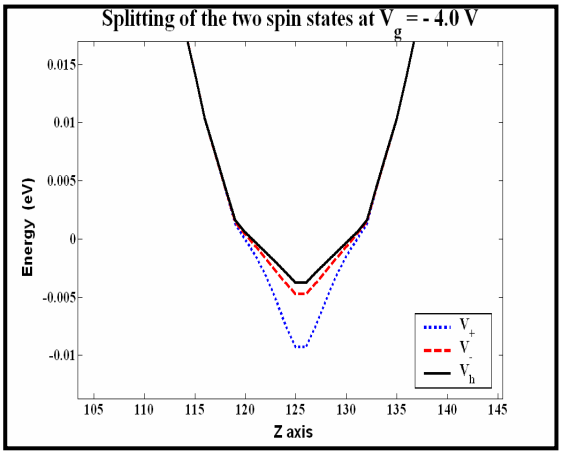

Figure 4: Energies of the Hartree, up and down spin electrons across the channel at V_g = - 4.0 V.

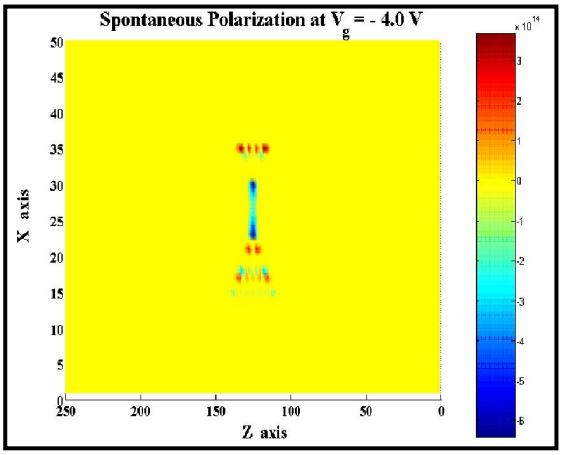

Figure 5: Spontaneous polarization ($n_- - n_+$) of the two spin states showing resonance states.

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