

One of the major challenges in the fabrication of quantum gates for quantum information processing is the ability to control efficiently the device parameters to insure reliable spin-qubit operation. This is particularly relevant in solid state technology with GaAs hetero-structure quantum dots where fluctuations in the materials parameters, device design and voltages should be reduced for allowing the proper sequence of C-NOT operations. In this context, the capability to understand the inter-relation between many-body effects and the device structure and operation is paramount.

We use quantum device modeling based on the 3D self-consistent solution of the Kohn-Sham equation within the local spin density approximation (LSDA) to describes the fine details of many-body interactions in 3D environment consisting of hetero-structures and different doping regions, with realistic boundary conditions [1]. The conditions for charging the dots with successive electrons, as a function of the applied gate biases, are determined by the Slater rule, which provides an elegant criterion for the dot energy stability. Hence, *microscopic* changes in the quantum states are described in terms of the variation of *macroscopic* parameters such as voltages, structure size and physical shape of the dots, without a-priori assumption on the quantum dot confining potential profile.

In this talk we shows that the design of quantum dot devices can be optimized for efficient spin-qubit operation. We successively consider two kinds of coupled quantum dots structures i.e. Laterally-Coupled Vertical Quantum Dots (LCVQD) [2] and Laterally-Coupled Planar Quantum Dots (LCPQD) [3] proposed to realize a C-NOT gate. In the latter design, two Quantum Point Contact (QPC) detectors placed in the vicinity of the double quantum dot enable the determination of the exact number of conduction electrons on each dot, starting with empty dots and progressively filling them with one electron at a time. In both cases, we obtained a comprehensive picture of the variation of the spin states and energy spectrum as function of the gate biases and device configuration. We are able to reproduce and optimize the response in the lateral QPC detectors to single electron charging in the individual dots of the LCPQD circuits. The addition energy and the voltage span for single electron charging are in excellent agreement with experiment. We also investigate the detector sensitivity of different QPC gate geometries to the first electron charging in the quantum dot [4]. For this purpose, we obtain the variation of the potential energy saddle point in the constriction at the first electron charging as a function of different QPC gate biases [Fig. 1(a)]. Based on the Buttiker formula [5], we then use this quantity to compute the relative change of the conductance ($\Delta G/G$) over the specified QPC gate bias range [Fig. 1(b)]. Our results indicated that constrictions with dented designs are more sensitive detectors than conventional QPC geometries.

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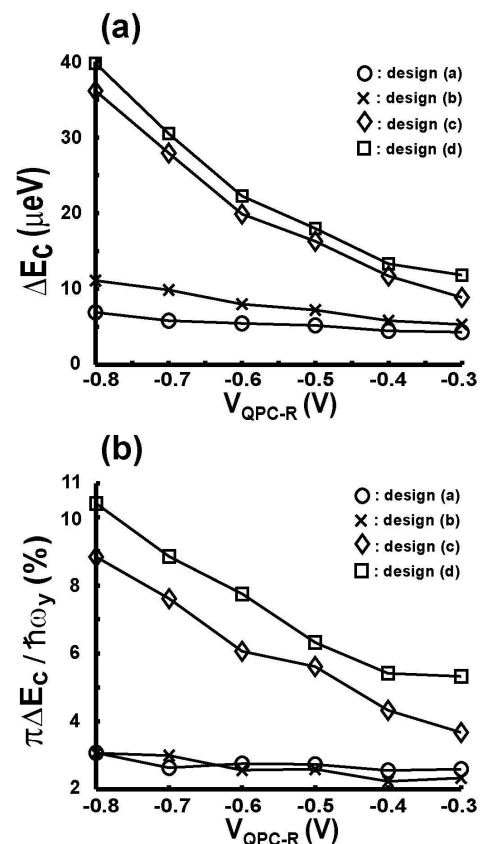


Figure 1. (a) Discontinuity of the saddle point of the potential energy in the confinement of the QPC ΔE_c as a function of QPC gate bias $V_{\text{QPC-R}}$ for four QPC designs (b) QPC sensitivity as a function of $V_{\text{QPC-R}}$. Designs (c) and (d) are dented geometries while designs (a) and (b) are conventional geometries