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# Electron-electron Interaction and Changing Effects in Semiconductor Quantum Dots

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## 1. Introduction

Zero-dimensional (0D) systems, such as quantum dots have been the subject of intense research in recent years because of novel fundamental physical phenomena as well as their potential for many exciting applications in optics and electronics. In this presentation, we discuss the influence of the confining potential and electron-electron interaction in the formation of shell structure in single quantum dots (QD), and the role of many body interaction, especially the effect of electron spin, on the charging behavior of coupled QDs. The electronic properties of the QDs are obtained by solving self-consistently the Schrödinger and Poisson equations on a three dimensional (3D) grid. The electron spin has been considered explicitly under the Local Spin Density Approximation (LSDA) in the density functional theory.

## 2. Quantum Dot Structures

Typical devices are shown in Fig. 1 (notice the *y*-axis is in the vertical direction). They consist of an inverted $GaAs/Al_{0.3}Ga_{0.7}As$ heterostructure which confines the electrons to a 2D gas at the interface. In our model, the simulated structure consists of a 22.5-nm layer of undoped $Al_{0.3}Ga_{0.7}As$ followed by a 125 nm layer of undoped GaAs and finally an 18 nm Ga as cap layer. The cap layer is uniformly doped to $5\times10^{18}$ $cm^{-3}$ so that the conduction band edge is just above the Fermi level at the GaAs-cap layer-undoped GaAs boundary. The inverted heterostructure is grown on a GaAs substrate and charge control is achieved by varying the voltage on the back gate, $V_{back}$.

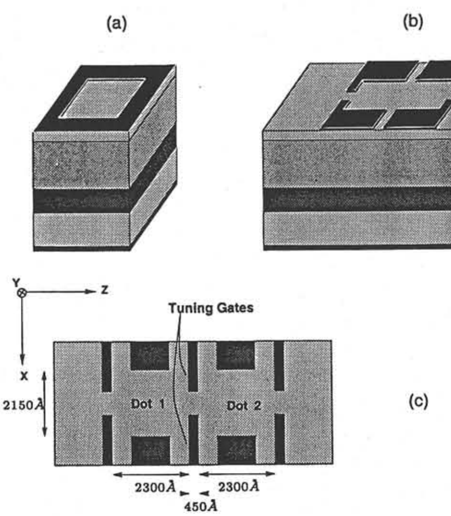


Fig. 1 Schematic representation of a) a square and b) a quad gate quantum dot device with layer structure c) Schematic representation along the $x-z$ plane.

The first quantum dot shown in Fig. 1.a. has a $240\times240$ $nm^2$ square open area at the top bordered by a 65-nm thick gate. The quad-gate device shown in Fig. 1.b. has four gate pads with 45-nm stubs protruding into the channel; the dimensions of the open area on the top are $230\times408$ $nm^2$. The separation between the pads along the (longer) *z*-direction is 90-nm. The schematic of the coupled dot structure is shown in Fig. 1.c. The two dots are defined by biasing the ten metallic gates, with the coupling between them varied by means of the voltage, $V_t$, on the tuning gates.

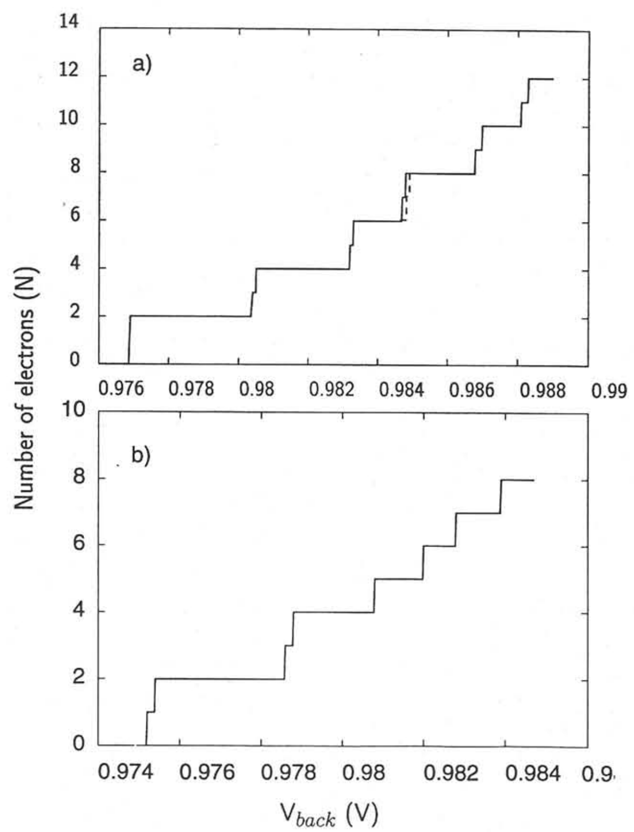


Fig. 2 Coulomb staircase diagram for the double-dot for a) The tuning gate $V_t$=−0.67 V. The transitions that do not follow Hund's rules are shown in dashed lines. b) $V_t$=−0.60 V.

## 3. Results

The single and coupled quantum dots show remarkable similarities to atoms and molecules. We observe that in the case of single quantum dots with cylindrical symmetry, the electrons in the dot form shells like in atoms. This shell structure is slightly distorted due to the electron-electron interaction, as the number of electrons, N, increases. If the dot is asymmetric, no pre-determined shell structure emerges except when Coulomb repulsion leads to accidental *Coulomb degeneracies*. In the case of coupled quantum dots, we observe that the dots can be driven from a state wherein the individual dots are separate, akin to two isolated atoms, to one in which the dots couple, forming an "artificial molecule." We show that both electrostatic and quantum mechanical coupling between the two quantum dots play a role in its charging properties, in accordance with experimental observations of Waugh *et al.*. We also show that when the inter-dot coupling is weak the lowest energy state is a spin polarized one, in accordance with Hund's rules. When the coupling is increased however, coherent *bonding* and *anti-bonding* states are formed which results in a termination of spin polarization. Furthermore, we find that for a strong inter-dot coupling the indirect exchange-mechanism induces ferromagnetic-like state.

## Acknowledgements

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