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M.Ghirlanda

Dipartimento di Ingegneria dell'Informazione: Elettronica, Informatica, Telecomunicazioni,
Università di Pisa

M. Governale

Dipartimento di Ingegneria dell'Informazione: Elettronica, Informatica, Telecomunicazioni,
Università di Pisa

Massimo Macucci

Dipartimento di Ingegneria dell'Informazione: Elettronica, Informatica, Telecomunicazioni,
Università di Pisa

Giuseppe Iannaccone

Dipartimento di Ingegneria dell'Informazione: Elettronica, Informatica, Telecomunicazioni,
Università di Pisa

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M. Girlanda,^{a)} M. Governale, M. Macucci, and G. Iannaccone
Dipartimento di Ingegneria dell'Informazione, Università di Pisa, 2, I-56126 Pisa, Italy

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We present evidence that operation of quantum cellular automaton (QCA) cells with four dots is possible with an occupancy of $4N+2$ electrons per cell (N being an integer). We show that interaction between cells can be described in terms of a revised formula for cell polarization, which is based only on the difference between diagonal occupancies. We validate our conjectures with full quantum simulations of QCA cells for a number of electrons varying from 2 to 6, using the configuration–interaction method. © 1999 American Institute of Physics.
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The concept of logic circuits based on quantum cellular automata (QCA), first proposed by Lent, Tougaw, and Porod,¹ has received much attention in the last few years, due to the perspectives of extremely low-power operation and to the drastic reduction of interconnections it would allow. The basic QCA building block is represented by a bistable cell made up of four quantum dots or metallic islands at the vertices of a square and containing two electrons that can align along the two different diagonals, thus encoding the two logical states. For an isolated cell, alignment along either diagonal is equally likely, but, in the presence of an external electric field such as that due to a nearby cell (driver cell in the following), in which polarization along one of the diagonals is externally enforced, also the electrons in the driven cell will align along the same diagonal, thereby minimizing the total electrostatic energy. It is, therefore, possible to propagate the polarization state along a chain of cells and it has been shown² that all combinatorial logic functions can be performed by properly designed two-dimensional arrays of such cells.

Various implementations of QCA cells have been proposed so far, based on metal islands,^{3,4} on quantum dots obtained in semiconductor heterostructures,⁵ or on nanostructured silicon islands.⁶ All of these implementations share the same problem: an extreme sensitivity to fabrication tolerances and the associated need for careful adjustment of each single cell. Such a sensitivity is the direct consequence of the smallness of the electrostatic interaction between nearby cells and, therefore, of the energy splitting between the configurations corresponding to the two logic states. While for the purpose of large-scale integration new approaches are needed, such as, possibly, resorting to implementations on the molecular scale, experiments for the assessment of the basic principle of operation are being performed by carefully tuning the voltages applied to adjustment electrodes built in each cell. The understanding that could so far be gathered from the existing literature was that strongly bistable and effective QCA operation was possible only in two regimes: either for cells containing just two

electrons² (and this would be the case for semiconductor quantum dots) or for cells containing two excess electrons on top of a very large total number of electrons, and operating in the classical Coulomb blockade limit.⁷

Based on the generally used expression for cell polarization P given in Ref. 1,

$$P = \frac{\rho_1 + \rho_3 - \rho_2 - \rho_4}{\rho_1 + \rho_2 + \rho_3 + \rho_4}, \quad (1)$$

operation was disrupted as soon as the number of electrons n per cell was other than two (ρ_i is the charge in dot i , and dots are numbered clockwise). For $n > 2$ the maximum polarization reached by the driven cell decreases, due to the fact that, while the denominator of Eq. (1) is nq , where q is the electron charge, the numerator at most reaches a value of $2q$. Indeed, a configuration with an excess of more than two electrons along one of the diagonals is not energetically favored for any reasonable arrangement of neighboring cells.

We observe that each cell is globally neutral, because electron charges are compensated for by ionized donors and by the positive charge induced on the electrodes defining the quantum dots. Such neutralization takes place over a certain region of space, with a finite extension. Therefore, even though the global monopole component of the electric field is zero, some effects proportional to the total number of electrons contained in the cell exist, but they are much weaker than those of the uncompensated “dipole” component associated with the asymmetry between the two diagonals, at least for most configurations of practical interest. This has led us to proposing a somewhat different expression for cell polarization, in which the denominator is always $2q$, independent of total cell occupancy:

$$P = \frac{\rho_1 + \rho_3 - \rho_2 - \rho_4}{2q}. \quad (2)$$

We argue that Eq. (2) provides a more realistic representation of the action of a cell on its neighbors than Eq. (1).

If the positive neutralizing charges were in the very same plane as that of the cell, and localized in each dot in an amount corresponding to $nq/4$, as in Ref. 2, our statement that only the difference between the numbers of electrons

^{a)}Electronic mail: mich@pimac2.i.et.unipi.it

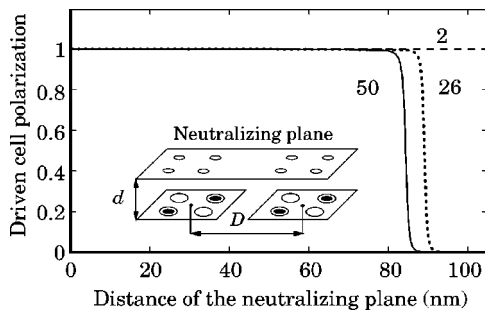


FIG. 1. Polarization of the driven cell as a function of the distance d between the cell and the neutralizing charge plane, for 2, 26, and 50 electrons, and a 0.7 polarization of the driver cell.

along the two diagonals matters would be rigorous, because the net charge in each dot is the same as in the case of a two-electron cell, in any realistic case.

The situation changes somewhat if the neutralizing charge is not located in the same plane as that of the cell electrons and/or is not equally distributed among the dots. In order to show that, in practical operating conditions, Eq. (2) still provides the best description of the polarizing action of a cell, we have studied two specific limiting cases: (a) neutralization by means of four $nq/4$ charges located in correspondence with the dots, but on a plane placed at an arbitrary distance d from the cell; and (b) neutralization by means of image charges located on a plane at an arbitrary distance h from that of the cell (such as in the case of Dirichlet surface boundary conditions at a distance $h/2$).

We have first considered a driver cell with a variable number of electrons, coupled to a driven cell with just two electrons, and investigated the polarization of the latter cell as a function of the polarization of the former [defined according to Eq. (2)]. For simplicity, we have assumed classical point-like charges in the driver cell, while a full quantum-mechanical solution has been performed for the driven cell, by means of the configuration–interaction (CI) method.⁸ The CI technique is based on expanding the many-electron wave function into a linear combination of Slater determinants built starting from a single-electron basis. The coefficients of this linear combination are the unknowns of the problem and can be determined by solving an algebraic eigenvalue problem,⁸ with a dimension corresponding to the number of Slater determinants that are taken into consideration. We assumed, for the driven cell, a confinement potential generated in a GaAs/AlGaAs heterostructure at a depth of 70 nm by a metal gate with four 90 nm holes with centers located at the vertices of a 110 nm square, considering an applied voltage of -0.5 V. The distance D between cell centers is 300 nm.

Let us first examine case (a): in Fig. 1 we report the polarization of the driven cell, in response to a 0.7 polarization of the driver cell, as a function of d for 2, 26, and 50 electrons in the driver cell. If there is a total of just two electrons, the driven cell is always fully polarized, independently of the distance at which the neutralizing charges are located. When the number of electrons becomes larger, the polarization of the driven cell is unaffected, as long as the neutralizing charges are within a reasonable distance from the driver cell; above a certain threshold value for d (depending on n), the locally uncompensated repulsive action of the

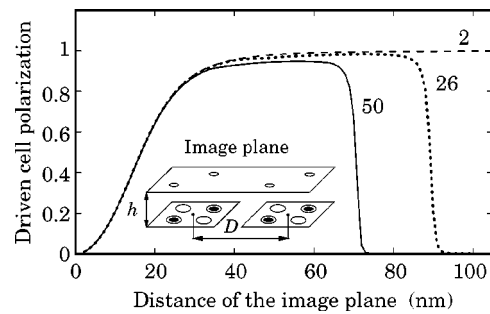


FIG. 2. Polarization of the driven cell as a function of the distance h between the cell and the image charge plane for 2, 26, and 50 electrons, and a 0.7 polarization of the driver cell.

electrons in the driver cell prevails and forces the electrons of the driven cell into the two rightmost dots, thus yielding zero polarization.

As far as case (b) is concerned, in Fig. 2 results are shown for 2, 26, and 50 electrons, for the previously described operating conditions. For large enough values of h , the polarization of the driven cell drops down to zero, because of the repulsive action of the locally uncompensated charge. In addition, the polarization decreases (in the same fashion, regardless of the number of electrons) for decreasing h : this is easily understood considering that the image charges do screen the action of the driver cell and such screening becomes more effective as the image plane approaches the cell plane.⁸

In Fig. 3 we report the complete cell-to-cell response function, i.e., the polarization of the driven cell versus that of the driver cell, for neutralization with image charges at a distance of 70 nm, and for 2, 26, and 50 electrons. Full polarization is reached both for 2 and 26 electrons, with some problem appearing for 50 electrons, that could be overcome adjusting the geometrical parameters.

Realistic situations are somewhere in between the two cases we have just discussed, since neutralization is performed by means of charges located both at the surface (metal gates or surface traps) and in the layers of the heterostructure. These results confirm the ability of our Eq. (2) to properly describe the polarizing action of a many-electron driver cell, and we can move on to the discussion of the response of a many-electron driven cell.

For this purpose, we can initially use an intuitive electrostatic model, in order to gain an immediate understanding of the problem, which will then be validated with a detailed quantum-mechanical calculation. We consider electrons as

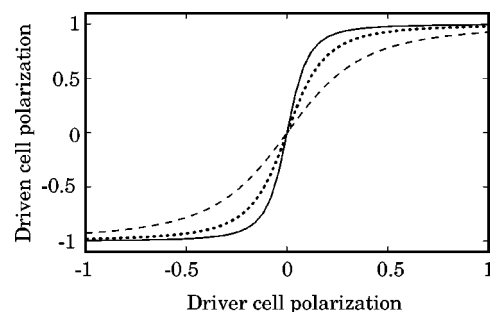


FIG. 3. Cell-to-cell response function for 2, 26, and 50 electrons in the driver cell.

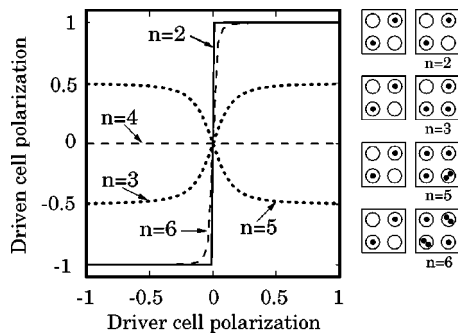


FIG. 4. Cell-to-cell response function for a driven cell with 2, 3, 4, 5, and 6 electrons, and sketch of dot occupancy.

classical particles, interacting via Coulomb repulsion, but with the possibility of tunneling between dots belonging to the same cell. The driver cell is assumed to have just two electrons and we examine the response of a many-electron driven cell. The configurations corresponding to the minimum electrostatic energy for cells with 3, 4, 5, and 6 electrons are shown to the right of Fig. 4. It is apparent that, while for 3 and 5 electrons the maximum polarization is only one half, and for 4 electrons is zero, for 6 electrons we obtain full polarization and a behavior that is substantially equivalent to that of a two-electron cell.

In order to validate this result, we have performed a quantum-mechanical calculation on cells containing up to 6 electrons, by means of the CI technique. While for up to 4 electrons a basis of just 4 single-electron wave functions is adequate for obtaining very accurate results, for 5 or more electrons a larger basis is in general needed, because the presence of two electrons in the same dot leads to a significant deviation from the single-electron wave functions. An acceptable approximation for the cases of interest can still be obtained with a total of 8 spin orbitals; significant improvements in the accuracy require a large increase in the number of determinants and are beyond the scope of the present work.

In Fig. 4 we report the CI results for the cell-to-cell response function of driven cells with 2, 3, 4, 5, and 6 electrons for barriers separating the dots higher than in the previous cases (this time the voltage applied to the gate is -0.7

V): the achieved limiting polarization values are in exact agreement with the predictions from the previously presented simple electrostatic model. In addition, we notice that around the origin the curve for a two-electron cell is steeper than that for the six-electron cell: this is due to the fact that the two “excess” (with respect to 4) electrons in the six-electron cell can be thought of as “seeing” a more shallow confinement potential, resulting from that of the two-electron cell plus the electrostatic action of the first four electrons. Such an effect can be compensated for by raising the potential barriers separating the dots of each cell.

From the intuitive electrostatic model and from the other results just described, we can conclude that QCA cell operation is substantially associated with the electrons in excess with respect to a multiple of 4: a six-electron cell yields full polarization as a two-electron cell; the same occurs for a ten-electron cell, and, in general, whenever the total number of electrons per cell equals $4N+2$, with N an integer.

This conclusion completes our understanding of the behavior of QCA cells, filling the gap between the operation with just two electrons^{2,8} and that in the metallic limit, with a very large number of electrons and two excess charges.⁷ Cells with $4N+2$ electrons are thus suitable for QCA operation, thereby lowering the technological fabrication requirements; however, symmetry constraints are in no way reduced as a result of the present findings, and remain the main obstacle preventing the implementation of practicable QCA logic.

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