

Configuration-interaction based simulation of a quantum cellular automaton cell

M. Girlanda

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

Configuration-Interaction Based Simulation of a Quantum Cellular Automaton Cell

M. Girlanda, M. Governale, M. Macucci, G. Iannaccone

Dipartimento di Ingegneria dell'Informazione, Università degli Studi di Pisa
Via Diotisalvi, 2 I-56126 Pisa, Italy
Phone: +39 050 568537 FAX +39 050 568522, E-mail massimo@mercurio.iet.unipi.it

We have investigated the behavior of a quantum cellular automaton cell made up of four quantum dots, in response to the electric field due to a nearby driver cell. We have implemented a simulation based on the single-shot Configuration Interaction technique, and we have studied the behavior of the cell for a number of electrons variable between 2 and 6. Our results support the conjecture that proper QCA operation can be obtained with a number of electrons per cell corresponding to $4N + 2$.

1. Introduction

Logic circuits based on the Quantum Cellular Automaton (QCA) concept have been proposed in the past few years[1] and their implementation with basic cells made up of four quantum dots is being pursued. Early calculations showed that optimal performance was obtainable with the total occupancy of a cell corresponding to two electrons[2] or, in the limit of metallic dots[3], with a very large number of electrons, but only two "excess electrons". On the basis of simple electrostatic considerations, we have developed the conjecture that proper operation can be achieved whenever the number of electrons in a cell equals $4N + 2$, with N integer.

We divide each cell into four quadrants, numbered counterclockwise, and we define the polarization P of a cell as

$$P = \frac{Q_1 + Q_3 - Q_2 - Q_4}{2}, \quad (1)$$

where Q_i is the integral of the electron density within the i -th quadrant of the cell. This expression for the polarization is different from that presented in [1] and [4]. We believe that such an expression is more suitable to the description of the operation of coupled cells containing an arbitrary number of electrons, because, if charge neutrality is achieved in each cell, the only significant coupling between neighboring cells is due to the electric dipole momentum created by the difference between the charge present along the two diagonals. For example, the driving action of a cell with one electron in dots 1 and 3, and with no electron in the other dots is substantially equivalent to that of a cell with two electrons in dots 1 and 3 and one electron in the other dots.

In a cell containing two electrons we can achieve po-

larization values ranging from -1 to +1, since the two electrons will align along one of the two diagonals, depending on the polarization of the driver cell. If the number of electrons is increased to 3, they will localize in three different dots; therefore, the difference between the total charges along the two diagonals cannot be more than 1 in modulus, and, as a consequence, the maximum cell polarization can range only from -0.5 to +0.5. With four electrons per cell no polarization can be achieved (unless an extremely strong external electric field is applied), because in the ground state configuration each dot will contain one electron and a configuration with two electrons in a single dot would correspond to a much higher electrostatic energy. With five electrons the situation is analogous to that with three electrons, with the only difference that there will be a dot with two electrons instead of an empty dot, and also in this case the polarization will range between -0.5 and +0.5. Finally, with six electrons two dots along one of the diagonals (the diagonal parallel to that with larger charge in the driver cell) will contain two electrons each, while the other two dots will contain a single electron. Thus the polarization will vary between -1 and +1, as in the case of a total cell occupancy of two electrons.

This conjecture, developed on the basis of an extremely simplified classical model, needs to be tested with a fully quantum mechanical calculation, which can also provide information about the actual shape of the polarization curve.

2. Model

We consider a GaAs/AlGaAs heterostructure and compute the cell confinement potential with a semi-

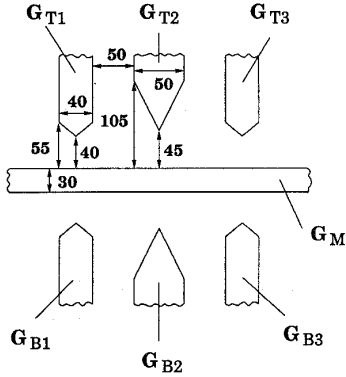


Figure 1: Gate layout of the QCA cell

analytic model, from the shape of the depletion gates and the applied bias voltages. The gate layout is represented in Fig. 1, with all dimensions expressed in nanometers. The distance of the two-dimensional electron gas (2DEG) from the semiconductor surface is 50 nm. The problem is treated within a 2-D approximation, in the hypothesis that the vertical thickness of the 2DEG (from which the quantum dots are obtained) is much smaller than the transverse size of the dots themselves. Due to the presence of quasi-degenerate states, a treatment based on iterative approaches relying on some sort of mean field approximation (Hartree, Hartree-Fock, Local Density Functional) cannot be successfully applied, because convergence is extremely difficult to attain, with the charge bouncing between configurations with almost identical energy.

For an artificial molecule such as a four-dot cell, the Configuration-Interaction (CI) technique [5], developed in the field of molecular chemistry, appears to be most appropriate. The many-electron wave function is represented as a linear combination of Slater determinants onto which the Hamiltonian of the problem is projected.

The Hamiltonian of our model reads

$$H = -\sum_i \frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{4\pi\epsilon} \sum_i \sum_{j<i} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} - \frac{1}{4\pi\epsilon} \sum_i \sum_{j<i} \frac{e^2}{\sqrt{|\vec{r}_i - \vec{r}_j|^2 + (2z)^2}}, \quad (2)$$

where $m = 0.067m_0$ (m_0 is the free electron mass), $\epsilon = \epsilon_r\epsilon_0$ ($\epsilon_r = 12.9$ and ϵ_0 is the vacuum permittivity), e is the electron charge, and z is the distance between the 2DEG and the semiconductor-air interface. The second term in the right hand side of Eq (2) represents the electrostatic interaction between each pair of electrons, while the third term represents the contribution of the image charges[4].

We represent each eigenfunction of the N -electron Hamiltonian as a linear combination of Slater determi-

nants built from a basis of single-electron wave functions:

$$\Psi = \sum_{k=1}^{\infty} c_k \Phi_k. \quad (3)$$

In practice, we must restrict ourselves to a finite number of Slater determinants, in order to make the problem computationally viable, and the coefficients c_k can be found as elements of the eigenvector \mathbf{c} in the secular equation $\mathcal{H}\mathbf{c} = E\mathbf{c}$, where the matrix \mathcal{H} is the representation of the Hamiltonian over the basis of Slater determinants chosen for the expansion of the N -electron wave function.

If we start from a set of M spin-orbitals, corresponding to a basis of $M/2$ single-electron orbitals, the number \mathcal{N}_{SD} of Slater determinants making up our basis will be given by

$$\mathcal{N}_{SD} = \binom{M}{N}. \quad (4)$$

where N is the number of electrons being considered. The size of the eigenvalue problem is therefore $\mathcal{N}_{SD} \times \mathcal{N}_{SD}$. It is possible to show that a certain fraction of the elements of \mathcal{H} are zero and selection rules can be derived to determine them[4]. These selection rules do not lead, however, to an appreciable reduction of the order of magnitude of the required computational effort. It is apparent from Eq. (4) that the size of the problem grows combinatorially with increasing M , which forces us to use reduced sets of spin-orbitals or to devise methods for the subsequent reduction of the number of Slater determinants.

The operation of a two-electron cell has been investigated in detail in Ref. [4]. In the case of just two electrons, a basis of four single-electron orbitals is sufficient to obtain accurate results for the cell-to-cell response function, since each dot contains at most one electron, and the electrostatic interaction between different dots is not large enough to significantly perturb the single-electron orbitals. In the present paper we are mainly concerned with a cell containing six electrons, in order to prove the previously mentioned conjecture based on a simple electrostatic analysis. With six electrons, there will be dots containing two electrons, where the electrostatic interaction will play an important role. An appropriate representation of the six-electron wave function would therefore require the expansion over a basis of Slater determinants built from more than just 4 basis functions. Due to symmetry properties, the next larger meaningful basis is made up of 12 functions, corresponding to 24 spin-orbitals. This leads to $\mathcal{N}_{SD} = 134,596$, thus to an eigenvalue problem which cannot be handled on a normal workstation.

In order to obtain a preliminary description of the behavior of a six-electron cell, we have therefore first approached the problem using a basis made up of just four single-electron basis functions.

3. Full CI results

We have computed the confinement potential produced by the gate layout of Fig. 1 by applying the semi-

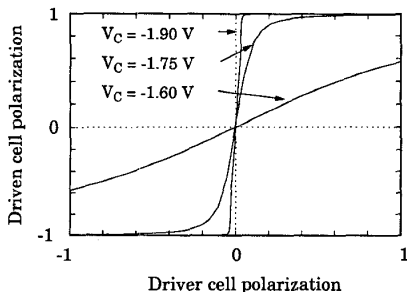


Figure 2: Polarization curves for three different values of the voltage applied to gates G_{T2} and G_{B2} .

analytical procedure described in Ref. [4], for three values of the voltage applied to gates G_{T2} and G_{B2} (-1.6 , -1.75 and -1.9 V) and a constant voltage of -1.8 V on the remaining gates. We have then performed a full CI calculation (i.e. no procedure to discard any of the determinants of the space generated from the chosen basis functions has been applied) with 28 Slater determinants, obtaining the cell-to-cell response function for a total cell occupancy of six electrons (see Fig. 2). In this case, as well as for all the other results presented in the following, the distance between the centers of the driver and the driven cell is assumed to be 300 nm, and the driver cell is always a two-electron cell (it is clear that a fully polarized six-electron cell would have substantially the same driving effect as a fully polarized two-electron cell).

The voltage on G_{T2} and G_{B2} determines the height of the potential barrier between the two upper and lower dots, respectively. The higher this barrier, the more localized the electrons will be, and therefore the steeper the polarization curve.

Results for different total cell occupancy are shown in Fig. 3, for a choice of -1.9 V for the voltage applied to G_{T2} and G_{B2} . We observe that for 2 and 6 electrons we obtain complete polarization, as expected. For three and five electrons the polarization of the driven cell remains at -0.5 or $+0.5$ for most values of the driver cell polarization, with a sharp transition around the origin. We notice that the sign of the polarization for three electrons is opposite to that for five electrons. The reason for this difference can be understood from a further examination of the classical electrostatic model: in both cases the “spare” electron will go in the corner of the driven cell furthest from the electrons in the driver cell and belonging to the diagonal orthogonal to that occupied in the driver cell. Thus, for $+1$ polarization in the driver cell, the polarization in a three-electron driven cell will be given by $P = (2 - 1)/2 = 0.5$, while that in a five-electron cell will be $P = (2 - 3)/2 = -0.5$. As expected, the polarization of the four-electron cell is zero for any value of the driver cell polarization.

The electron density in the driven cell for $P = +1$ is reported in Fig. 4 for three electrons (Fig. 4(a)), five

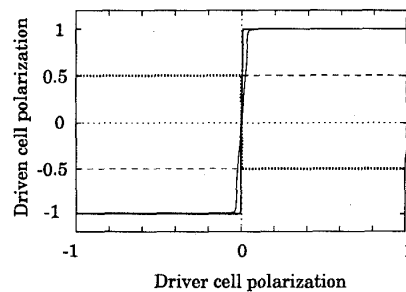


Figure 3: Polarization curves for a total cell occupancy of two (thick solid line), three (dashed), five (dotted) and six electrons (thin solid).

electrons (Fig. 4(b)), and six electrons (Fig. 4(c)). The behavior of the electron densities confirms the previously presented discussion based on classical arguments.

4. Determinant selection technique

As already mentioned, it seems inadequate to simulate the presence of six electrons in a cell starting from a basis which contains less than 12 one-electron orbitals. On the other hand, the number of Slater determinants grows combinatorially with the number of electrons and of basis functions used for building them. For six electrons and 12 basis functions, the size of the full CI space (i.e. the total number of determinants) is already of the order of several hundred thousand. Therefore, in order to make the problem computationally manageable, we have developed a technique to reduce the size of the CI space without, however, losing accuracy.

We have chosen a zeroth-order space (\mathcal{S}_l) containing 4 Slater determinants obtained by selecting the ones with the four largest coefficients in the ground-state wave function expansion out of the 28 determinants generated with the four lowest-energy basis functions. Then, for each determinant Φ_k of the full space, we have computed the quantity σ_k thus defined

$$\sigma_k = \frac{|\langle \Phi_0 | \hat{H} | \Phi_k \rangle|^2}{|\varepsilon_0 - \varepsilon_k|}, \quad (5)$$

where $\Phi_0 \in \mathcal{S}_l$ and $\varepsilon_i \equiv \langle \Phi_i | \hat{H} | \Phi_i \rangle$.

Finally, we have retained the determinants for which σ_k is greater than a given threshold. Through successive reductions of the threshold value, we can move from the zeroth order space to the full CI space (corresponding to a zero value for the threshold), spanning a wide collection of different-sized spaces.

We have included up to about a thousand determinants, until further enlargements of the CI space did not appear to affect the results. Preliminary data for the response function of a six-electron cell are reported in Fig. 5, where the curve obtained with 780 Slater determi-

nants has been plotted together with that resulting from a full CI calculation with 28 determinants. The confining potential with the gates G_{T2} and G_{B2} kept at -1.6 V has been used.

The dashed curve in Fig. 5 corresponds to the response function (computed with a full CI basis of 28 determinants) of a two-electron cell defined by the same confining potential. It is possible to provide an intuitive explanation of the reason why the six-electron curve is less abrupt than the two-electron one, on the basis of a simple Hartree picture. The abruptness of the polarization curve increases with increasing height of the barriers (which corresponds to an increase in the electron localization): the two electrons in excess with respect the four evenly distributed in the four dots experience a total potential that is the result of the confining potential plus the Hartree potential due to the other electrons. Such a potential has lower potential walls with respect to the bare confining potential seen by the electrons in the two-electron cell, and this leads to a less abrupt polarization curve.

5. Conclusions

A technique borrowed from molecular chemistry has been used for the simulation of coupled QCA cells containing a number of electrons varying between two and six. Full cell functionality has been obtained with two and six electrons, confirming a conjecture developed on the basis of electrostatic considerations. A critical issue is the reduction of the number of Slater determinants used for the expansion of the many-electron wave function, for which a selection technique has been developed. Encouraging preliminary results have been presented, while further work is needed to make the selection procedure more robust and reliable.

Acknowledgments

This work has been supported by the ESPRIT Project 23362 QUADRANT (QUAntum Devices for Advanced Nano-electronic Technology).

References

1. P. D. Tougaw and C. S. Lent, *J. Appl. Phys.* **75**, 1818 (1994).
2. P. D. Tougaw, C. S. Lent, and W. Porod, *J. Appl. Phys.* **74**, 3558 (1993).
3. C. S. Lent and P. D. Tougaw, *J. Appl. Phys.* **75**, 4077 (1994).
4. M. Governale, M. Macucci, G. Iannaccone, C. Ungarelli, J. Martorell, submitted to the *Journal of Applied Physics*, cond-mat 9804228.
5. R. McWeeny, *Methods of molecular quantum mechanics* (Academic Press, London, 1989) and references therein.

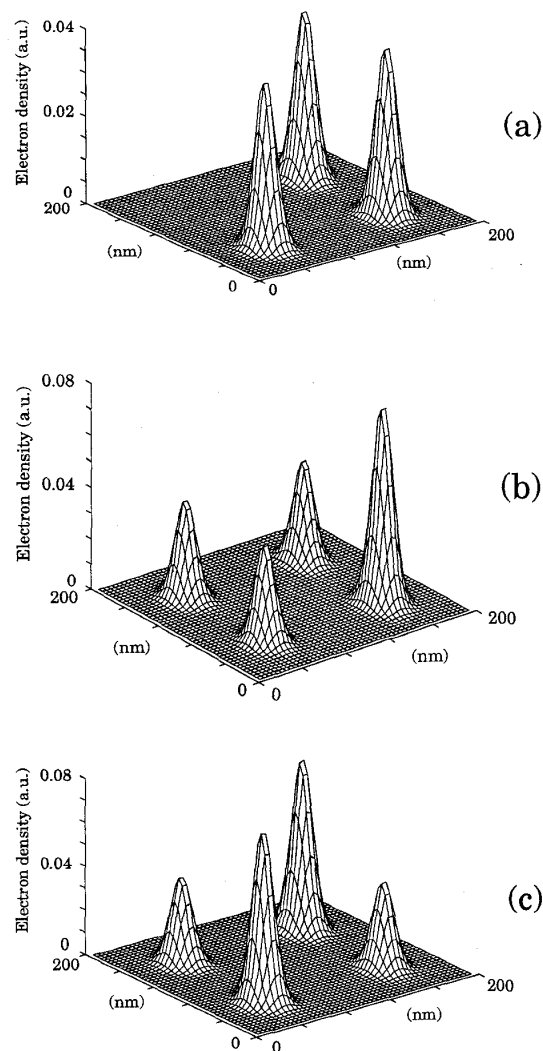


Figure 4: Electron density for $P = 1$ for a cell containing three (a), five (b) and six (c) electrons.

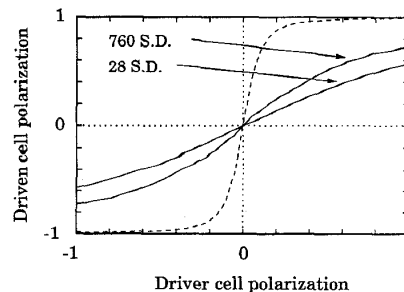


Figure 5: Polarization curves of a six-electron cell computed with a basis of 28 and 780 Slater determinants (solid lines) and of a two-electron cell (dashed).