

# Self Consistent Quantum Mechanical Modelling of QCA

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**ABSTRACT:** A self consistent quantum mechanical modelling using Hartree-fock approximation technique for Quantum-dot cellular automata (QCA) is proposed in this work. The wavefunctions and energy levels of the SEF in QCA cell and its effects on subsequent QCA cells are presented. It is observed that the polarity of the subsequent QCA cell is inverted when compared to the normal case due to presence of Single Electron Fault (SEF) in a QCA cell. A systematic methodology is presented to encounter this problem. The basic target of this paper is to present simple quantum mechanical modelling of QCA with tight-binding Hubbard-type Hamiltonian with coulombic repulsion model solved using Hartree-fock approximation.

**KEYWORDS:** Quantum-dot cellular Automata (QCA), Single Electron Fault (SEF), quantum dots, coupling of QDs, coulombic interaction.

## I. INTRODUCTION

Incredible growth in CMOS technology has brought it to a stage where researchers are looking for alternative of CMOS or CMOS with alternate structure (Gupta, Moroz, Smith, Lu, & Saraswat, 2014). Reasons include quantum mechanical behaviour of electron at low dimension, power dissipation, leakage currents, parasitic capacitances etc. In spite of using high K material at gate, the amplification factor is reducing tremendously with size. A paradigm shift with quantum devices is seemingly inevitable. QCA has emerged as a promising alternative to current CMOS VLSI. QCA is introduced to create nano-scale devices with high compaction density capable of performing computation at high switching speed. It was first proposed by Toffoli (Margolus & Toffoli, 1987) but the solid state structure was proposed by Lent et. al (Lent, Tougaw, & Wolfgang, Bistable Saturation in Coupled Quantum Dots for Quantum Cellular Automata, 1993). Initially, the structure was proposed with five QDs, but eventually it was established that very stable structure can be made using four QDs (Tougaw & Lent, 1996). Rigorous research is going on towards the implementation of complex logic structure in QCA (Pudi & Sridharan, 2011; Sridharan & Pudi, 2015; Sen, Dutta, Mukherjee, Nath, Sinha, & Sikdar, 2016).

A QCA is composed of array of interactive cells, each cell having four QDs arranged at four corners of the square shaped cell. The centre to centre distance between two cells is appreciably more than the distance of two QDs of same cell to avoid tunnelling of electron between cells. Every cell is assumed to have two electrons located diagonally due to coulombic interaction. The major interaction between the cells is coulombic force. Figure 1 shows the structure of the QCA cells. Position of electrons in subsequent cell are dependent on the position of electrons in preceding cell. This is how the polarization is propagated through the cells. Majority gate and inverter are the basic logical operations based on QCA (Lent, Tougaw, & Wolfgang, Bistable Saturation in Coupled Quantum Dots for Quantum Cellular Automata, 1993).

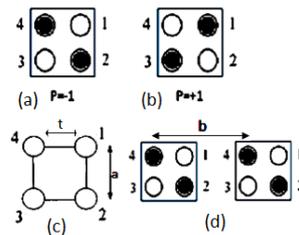
Nanoscale devices, like QCA, are susceptible to high error rate. The faults in QCA structure has become a significant area of research (Momenzadeh, Tahoori, Huang, & Lombardi, 2004; Anduwan, et al., 2010; Sen, Dutta, Mukherjee, Nath, Sinha, & Sikdar, 2016). The effect of temperature has been addressed and modelled since the introduction of QCA and still being discussed (Lent, Tougaw, & Wolfgang, Bistable Saturation in Coupled Quantum Dots for Quantum Cellular Automata, 1993; Anduwan, et al., 2010). Some of the faults and defects associated with QCA are stray charge defect, shifted device defect, missing cell defects, single electron fault, three electron fault, misshapen fault etc (Crocker, Hu, & Niemier, 2009). Since, the position of electron influences the signal transition and propagation, it is important to investigate all the physical faults related to electron and/or dot in QCA cells (Mahdavi, Mirzakuchaki, Moghaddasi, & Amiri, Single Electron Fault Modelling in Quantum Binary Wire, 2011; Mahdavi, Mirzakuchaki, Moghaddasi, & Amiri, Single Electron Fault Modeling in Basic Quantum Devices, 2011).

The problem of fault and fault tolerance in QCA structure is addressed by solving Hamiltonian, and most popular model is tight-binding Hubbard-type Hamiltonian with Coulomb repulsion which is usually solved using Hartree-fock method (Pfannkuche, Gudmundsson, & Maksym, 1993; Governale, Macucci, Iannaccone, & Ungarelli, 1999; Lent, Isaksen, & Lieberman, Molecular Quantum-Dot Cellular Automata, 2003). We found that a simpler method, with

added post simulation work, can be exploited. Presented model uses a very fast method proposed by R. Kosloff (Kosloff, 1986) which has been adapted for coupled QD systems (Badnarek, Effective Interaction for Charge Carriers Confined in Quasi-one-dimensional Nanostructures, 2003; Badnarek, Time-evolution Simulation of a Controlled-NOT Gate with Two Coupled Asymmetric Quantum Dots, 2005; Sinha, Kumar, & Kumar, 2015). We have used this imaginary time technique to obtain the energy eigenvalues and wavefunction for addressing a simple quantum mechanical modeling of SEF in QCA. The results obtained is compared with the results obtained with Hartree-Fock technique. Mahdavi et.al. also presented simple model for SEF, but that method used only electrostatic energy estimation (Mahdavi, Mirzakuchaki, Moghaddasi, & Amiri, Single Electron Fault Modelling in Quantum Binary Wire, 2011; Mahdavi, Mirzakuchaki, Moghaddasi, & Amiri, Single Electron Fault Modeling in Basic Quantum Devices, 2011; Mahdavi, Amiri, Mirzakuchaki, & Moghaddasi, 2010). However quantum mechanical modeling is expected to give better results at nanoscale. In this work we have described the QCA cell and its operation in section II. In section III, we have discussed the formulation of problem. Computational method has been described in section IV. We have presented the results for variation of positions of single electron in QCA and its effect on subsequent QCA in section V. Conclusions and an approach to tackle the effect of SEF are presented at last.

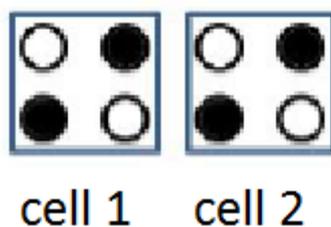
## II. DESCRIPTION OF QCA

Figure 1 gives schematic of the ideal QCA cell structures in ground state, which have four identical QDs represented as open circles, forming corners of a square. We assume two electrons, represented by solid dots, in each cell occupying the diagonal positions. The polarization is defined as given in figures 1(a) and (b), anticlockwise position to be -1 polarization ( $P = -1$ ) and clockwise position to be +1 polarization ( $P = +1$ ) respectively.



**Figure 1:** Ideal QCA cells, with (a) -1 polarization (b) +1 polarization, (c) dimensions of the cell (d) intercellular distance.

In a cell the electrons are allowed to jump between the individual QDs using quantum mechanical tunnelling. In an isolated cell the electron will occupy the diagonal dots at ground state due to the coulombic force possessing either of polarization. This gives a bistable latch like behaviour with only two stable states. The nearby cells have sufficient barrier in form of intercellular distance, to completely suppress the tunnelling to occur between adjacent cells. Coupling between two adjacent cells is governed by the coulombic interaction and clocking action. Figure 2 shows the coupling between the adjacent cells which compels cell 2 to have the same polarization as cell 1.



**Figure 2:** Cell 2 has the same polarization as cell 1 due to coulombic interaction.

The physical interaction between cells may be used to realize elementary Boolean functions. The basic logic gates using QCA structure are given in figure 3.

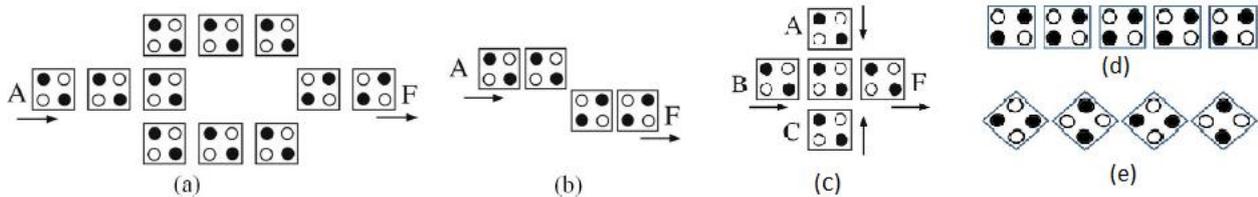


Figure 3: (a) Redundant inverter gate, (b) Inverter gate, (c) Majority logic gate, (d) Binary wire and (e) Inverter chain.

Majority logic function given in figure 3(c) is the most important logic gate, with which we can implement OR gate when one input is permanently fixed to logic 1, and AND gate can be implemented fixing one input to logic 0. Clocking is very important aspect of QCA, which not only provides a mean for synchronizing information flow along the circuit, but also controls the direction of information flow in a QCA circuit. The QCA clock also provides the power required for the logic operations. Actually, the clock is used to control the tunnelling barrier height of QD in a QCA cell. Clocking scheme can be divided into four regions as given in figure 4(a). When clock gets low, the electron gets trapped in QD and cannot tunnel to other QD. This is the hold phase. When the clock signal is high, all QD's barrier gets lower and electrons are free to move. This may be called to be null polarization state or relax phase.

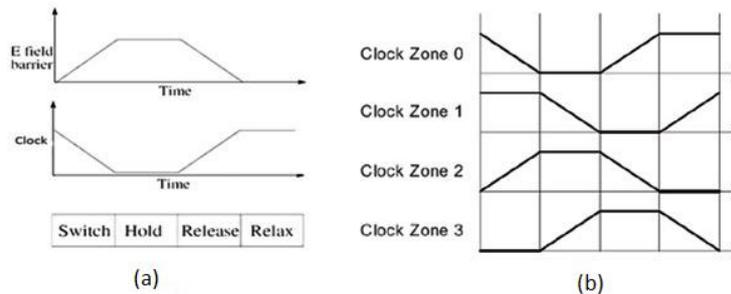


Figure 4: (a) Clocking scheme, clock regions and corresponding barrier potential, (b) QCA clock Zone

Figure 4(b) shows QCA clock, each cell in a particular clocking zone is connected to one of the four available phases of the QCA clock. Each cell in the particular clock zone is latched unlatched, and synchronized with the changing clock signal (Amiri, Mahdavi, & Mirzakuchaki, 2008).

### III. FORMULATION OF PROBLEM

We have taken QCA as described in figure 1 in last section. Figure 1(c) gives the dimensions of one cell. In our case the centre to centre distance between two neighbouring QDs,  $a=9\text{nm}$ , interdot distance  $t$  is  $4\text{nm}$ , and the dot diameter is  $5\text{nm}$ . The distance between the centres of two adjacent cells is  $20\text{nm}$  (let us call this distance to be 'b' for using it in equations). For example, considering two neighbouring cells, the distance between dot 4 in the left cell and dot1 in the right cell is  $29\text{nm}$ . We have taken InAs dots on GaAs substrate in our studies. The band offset between InAs and GaAs at conduction band is considered to be  $570\text{meV}$ . All dimensions are taken in AU for simulation. The confinement potential of QDs is considered to have Gaussian shape. Also we have assumed that, each cell is assigned to an individual clock zone and there are no neighbour cells in the same clock zone.

Here we are addressing Single Electron Fault (SEF), in which we assume that a single QCA cell in between the binary wire or inverter chain has only one electron as shown in figure 5. Figures 5(a) and 5(b) show the effect of SEF in binary wire and 5(c) and 5(d) shows the effect on inverter chain.

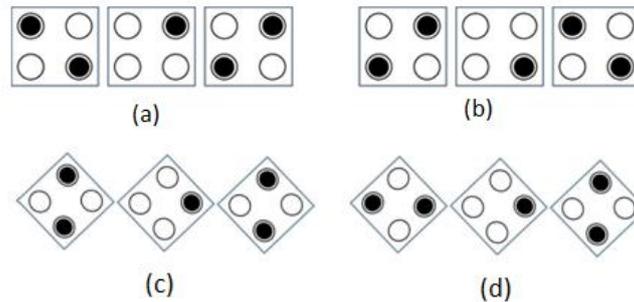


Figure 5: Single Electron Fault (a), (b) in binary wire, and (c), (d) in inverter chain.

We can observe that the effect of single electron logically inverts the expected result. It adversely affects the operations of QCA. To verify this result we must model the QCA cells using quantum mechanical modelling. In this paper we have proposed that the QCA structure can be modelled and simulated with a simple model and simpler method of solving Hamiltonian. This model has been used to address the single electron fault.

#### IV. METHOD OF SOLVING THE PROBLEM.

Here we are dealing with multiple electrons, a self-consistent loop for obtaining the wavefunction is needed because each particle sees the potential due to other. For such problems Hartree-fcok (HF) approximation has been used in addition to the imaginary time propagation technique. An important unsolved problem specifically in CNOT gate and QCA is how to deal with indistinguishable, interacting particles which determine the behaviour of electrons. The basic problem is that if particles interact, that interaction must be in the Hamiltonian. So until we know where the particles are, we can't write down the Hamiltonian, but until we know the Hamiltonian, we can't tell where the particles are. In HF approximation the idea is to solve the Schrödinger equation for an electron interacting with quantum dots and all the other electrons. The HF method can be viewed as a variational method in which the wave functions of the many-electron system have the form of an antisymmetrised product of one-electron wave functions (the antisymmetrisation is necessary because of the fermion character of the electrons). This restriction leads to an effective Schrödinger equation for the individual one-electron wave functions with a potential determined by the states occupied by the other electrons. We start with the electron charge density obtained by the imaginary time propagation technique and solve one-particle Schroedinger equations to obtain many electron wavefunctions. Then we construct the potential for each wavefunction from that the dots and that of all the other electrons, symmetrise it, and solve the one electron Schroedinger equations again. Fock improved on Hartree's method by using the properly antisymmetrised wavefunction (Slater determinant) instead of simple one-electron wavefunctions. Without this, the exchange interaction is missing. This method is suitable for a computer, because it is easily written as an algorithm.

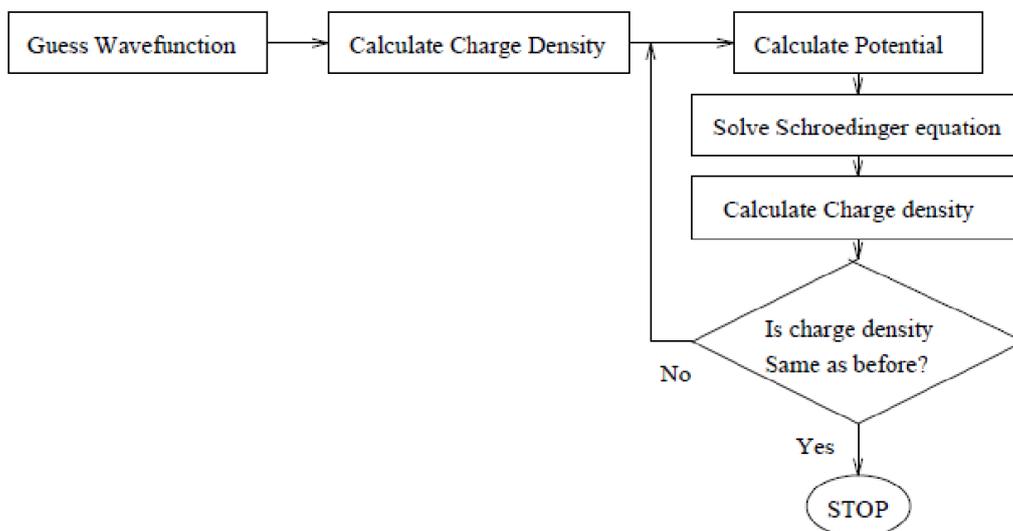


Figure 6: Algorithm for Self-consistent field theory.

Numerical method given by Jos Thijssen (Thijssen, 2007) has been adopted for the self consistent solution.

To optimize the result we first take a guess of wavefunction on a coarse grid and carry out propagation operation. The wavefunctions thus obtained is used as new assumption and is propagated on a finer grid. This can be done in recursion to optimize the result. Another optimization can be done with taking small propagating time initially and then repeat the process to avoid loss of normalization.

Now the wavefunction as obtained by the above procedure can provide the probability of electron found at any QD. Here we are assuming that when the clock is high (in relaxed phase for a given QCA cell) and the tunnelling height is lowered the electron has tendency to get to the QD with highest probability density. Following assumptions are made to simplify the model.

- I. We are concerned about the probability density and we have not modelled the presence of two or more electron in the cell. However special treatment is done to compensate this anomaly.
- II. We have not considered the spin state of electron.

The Hamiltonian of the specified cell includes the confinement potential of QDs and coulombic energy of the preceding cell. Hence the Hamiltonian of the second cell when first cell has polarization  $p = -1$ , is given by

$$-\frac{\hbar^2}{2m}(\partial_x^2 + \partial_y^2)\psi + V_{x,y}\psi = E\psi \tag{1}$$

where potential  $V_{x,y}$ , is given by

$$V_{x,y} = V_0 \exp\left[-\frac{a}{2}x - \frac{a}{2}y + \frac{q}{4}x^2 - \frac{b}{a} + \frac{a}{2}y - \frac{a}{2}y^2 + \frac{q}{4}y^2 - \frac{b}{a} + \frac{a}{2}y + \frac{a}{2}y^2\right] \tag{2}$$

Here  $a$  and  $b$  are dimensions as described in figures 1(c) and 1(d),  $\epsilon_{sc}$  is the relative permittivity of the semiconductor QD (This has to be added in recursion for coordinates  $x$  and  $y$ ). Using the technique described in this section the wavefunction and energy eigenvalue are deduced. From the wavefunction, we calculate the probability density of the electron at different QDs.

The wavefunction obtained by imaginary time propagation technique for single electron has been used as guess function in our work to save time of convergence.

The results are described in next section.

For simulations all the dimensions are taken in atomic unit (AU).

### V. RESULTS AND DISCUSSION

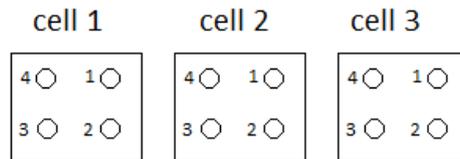


Figure 7: Three interacting QCA cells.

Following are the results of calculation of probability densities of electrons at different sites of a cell as given in the figure 7.

As more than one electrons are involved, a self consistent approach had to be used in addition. For single electron has been at site 1 in cell 2 the result obtained for cell 3 by HF method is given in Fig.8.

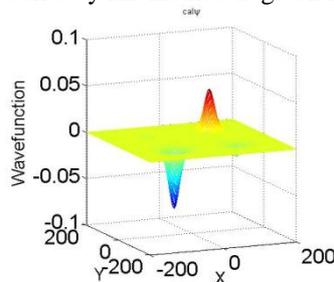
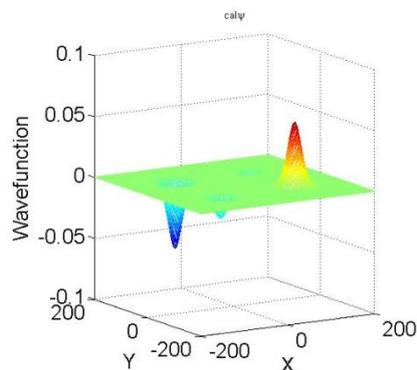


Figure 8: Wavefunction (calculated with HF method) for cell no. 3 when cell 2 has one electron at site 1.

Similarly, for single electron at site 2 in cell 2 the result obtained for cell 3 by HF method is given in Fig. (9):



**Figure 9:** Wavefunction (calculated with HF method) for cell no. 3 when cell 2 has one electron at site 2.

## VI. CONCLUSIONS

We have proposed a simple model for simulating QCA. Single electron fault is dealt in detail, which shows that it has an alarming effect. Other faults like effect of temperature, stray charge defect, shifted device defect, missing cell defects, single electron fault, three electron fault, misshapen fault can be modelled and simulated through this method. As a remedy to this problem, whenever we deal with binary wire we can have two more redundant wire and use majority gate at last before the next logic operation. This will decrease the probability of error in great extent.

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