

Quantum Mechanical Simulation of QCA with a Reduced Hamiltonian Model

Faizal Karim, Aryan Navabi, Konrad Walus and André Ivanov

Dept. of Electrical and Computer Engineering
University of British Columbia

Abstract—Molecular quantum-dot cellular automata (QCA) is an emerging computing paradigm which utilizes electrostatic coupling between electronic configurations in neighboring molecules to perform information processing. A simulation tool for this technology, QCADesigner, exists and allows designers to quickly layout and simulate QCA circuits constructed with up to thousands of QCA cells. However, in general, large quantum mechanical systems are not suitable for efficient simulation on a classical computer, and as a result, QCADesigner uses the Hartree-Fock approximation to reduce the computational complexity of the simulation. Under certain circumstances, this approximation can lead to the incorrect ground state and hence, produce logically incorrect results at the outputs. In this work, we provide examples of problem circuits and propose a method to identify areas that must be simulated using the full Hamiltonian.

I. INTRODUCTION

The QCA paradigm is one in which an array of cells, each electrostatically interacting with its neighbors, is employed in a locally interconnected manner [1]. Several proof-of-concept QCA devices have been fabricated using silicon-on-insulator (SOI) [2], metallic island implementations operating in the Coulomb blockade regime [3]–[9], and nano-magnetics [10]–[15]. In recent years, research into implementing these devices using single molecules has also begun to generate significant interest [16]–[22]. A simulation tool, QCADesigner, exists for this technology [23]–[26] and has been applied towards the high-level design and exploration of both sequential and combinational circuits [27]–[29]. QCA is a ground state computing paradigm which does not require coherence across the entire circuit. As such, QCADesigner is able to use the Hartree-Fock approximation to simulate QCA circuits in order to reduce computational complexity. However, it has been shown that this approximation can lead the simulation to settle to an incorrect ground state [30], [31], and hence, produce logically incorrect results at the outputs. This work address this issue and proposes an algorithm to identify the areas of the circuit that cannot be treated using the Hartree-Fock method.

II. BACKGROUND AND MOTIVATION

The Hartree-Fock method is an approximate method to determine the ground-state wavefunction and energy of a

many-body quantum system. Effects arising from quantum correlations in this approximation are neglected. In the intercellular Hartree-Fock approximation used in QCADesigner, an N -cell system is decoupled into a set of N single-cell subsystems that are assumed to interact classically through expectation values without any quantum mechanical coherence between neighboring cells [24]. Using this approximation, it is only necessary to solve N 2×2 Hamiltonians as opposed to one $2^N \times 2^N$ Hamiltonian. This allows large circuits, which would otherwise be intractable using a full quantum mechanical model, to be simulated on a classical computer [23]. One of the primary drawbacks of the Hartree-Fock method, and in particular, with respect to QCADesigner, is that neglecting quantum correlations can lead the simulation to settle to a meta-stable ground state. One such example is the majority gate described in [30], [31] and shown in Fig. 1. In this example, the majority gate has input legs of unequal length. One of the input legs is only one cell long and is coupled to driver cell, $P_{\text{driver}3}$, which has a polarization, $P = -1$. The other two input legs are each four cells in length and are driven by cells ($P_{\text{driver}1}$, $P_{\text{driver}2}$) each having polarizations, $P = +1$. Using the Hartree-Fock approximation, QCADesigner outputs the logically incorrect result at cell 11. In [30], [31], Toth suggests that this can be avoided by modeling the 5 cells in the “cross” region of every majority gate with a 5-cell Hamiltonian, and modeling the remaining cells using the Hartree-Fock method.

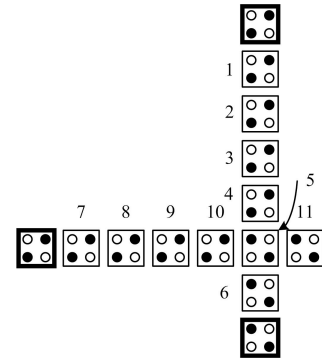


Fig. 1. Example of a majority gate for which QCADesigner produces the incorrect output using the Hartree-Fock approximation.

However, not all majority gates settle to a meta-stable ground state and hence solving the full Hamiltonian for those majority gates would require a needless increase in com-

F. Karim, A. Navabi, K. Walus and A. Ivanov are with the Microsystems and Nanotechnology Research Group at the University of British Columbia, Department of Electrical and Computer Engineering, 2332 Main Mall, Vancouver, BC, Canada V6T 1Z4 Phone: 604-827-3412, (e-mail: {faizalk,anavabi,konradw,ivanov}@ece.ubc.ca).

putational complexity. Moreover, modeling the cross region in every majority gate would require the simulation tool to provide predetermined blocks for the majority gate, not allowing the designer the freedom to layout circuits at will. Additionally, this problem is not only limited to the majority gate but can also be shown to occur in other QCA circuitry such as the layout shown in Fig. 2. In the latter, a long wire is experiencing crosstalk due to the presence of a single cell in a neighboring wire. In this scenario, the Hartree-Fock method results in cell 8 being so strongly influenced by the interfering cell, that it takes on a polarization as determined by this cell and not by the driver cell, as would be expected from solving the full Hamiltonian for the system.

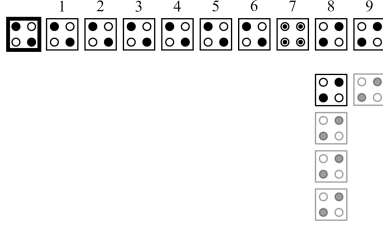


Fig. 2. Example of a wire experiencing crosstalk for which QCADesigner produces the incorrect output using the Hartree-Fock approximation.

III. CONTRIBUTION

The two aforementioned factors highlight the need for an algorithm to be developed that targets all the cells in a given circuit whose correlations to neighboring cells can no longer be considered negligible, and then models only those groups of cells using separate multi-cell Hamiltonians. To this effect, we propose a rudimentary algorithm that pre-determines these groups of cells based on the layout of the QCA circuit and then refines these groups - post-simulation - using two-point correlations. The pseudo-codes for both of these algorithms are shown in Figs. 3 and 4. In Algorithm 1, the input to createHam() is a circuit, C . In the algorithm, the total intercellular coupling, E_k , for each cell in C is computed and compared to a threshold value to determine whether or not the cell should be included in a separate Hamiltonian. If a given cell, c , is not within a radius, r , of any of the existing cells in $cell_group(i)$, then it is checked against the next cell group, $cell_group(i+1)$, and so on until a cell group is found. If no existing cell group contains any cells within the specified radius, a new group is formed beginning with cell, c . Once every cell has been observed, all cell groups are collected into H_group . H_group now consists of all the groups of cells that will require a separate Hamiltonian during simulation. In the second algorithm, regroupHam() takes in the previously found H_group as its input, and uses the following two-point correlation proper equation found in [30] to further refine H_group :

$$M_{zz}(i, j) = K_{zz}(i, j) - \lambda_z(i)\lambda_z(j), \quad (1)$$

where $K_{zz}(i, j)$ is the two-point correlation term between cells i and j , and λ_z is the single-cell coherence term. K_{zz} and λ_z can be found by computing [30],

$$K_{zz}(i, j) = \langle \sigma_z(i) \sigma_z(j) \rangle, \quad (2)$$

and [30],

$$\lambda_z = \langle \sigma_z \rangle, \quad (3)$$

respectively, where σ_z is the Pauli- z spin matrix and $\langle \sigma_z \rangle$ denotes the expectation value of the operator. If for two given cells, c_1 and c_2 , the M_{zz} term is above the specified threshold, then both c_1 and c_2 are kept in their current cell grouping. If any cell is not highly correlated to any of its neighbors, then it is removed from the cell group and refinement is achieved.

Algorithm 1 createHam(C)

```

1:  $E_k^0$  = Kink energy between two neighboring cells (intercellular coupling);
2:  $\delta$  = threshold value;
3:  $r$  = radius of effect;
4: while there exists unobserved cells in  $C$  do
5:    $i = 1$ ;
6:    $c$  = a cell in  $C$  that has not been observed;
7:    $|E_k^0|$  = sum of the kink energies between cell  $c$  and all other cells in  $C$ ;
8:   if  $E_k^0 > 2|E_k^0| + \delta$ ;
9:     while  $i \leq$  total number of cell groups do
10:      if distance between cell  $c$  and any cell in  $cell\_group(i) \leq r$ ;
11:        place cell  $c$  in  $cell\_group(i)$ ;
12:        break;
13:      else
14:         $i++$ ;
15:      end if
16:    end while
17:    if  $i ==$  total number of cell groups;
18:      place cell  $c$  in  $cell\_group(i+1)$ ;
19:    end if
20:  end if
21: end while
22:  $H\_group = cell\_group$ ;
23: return  $H\_group$ ;
```

Fig. 3. Pseudo-code for grouping together cells with large E_k .

Algorithm 2 regroupHam(H_group)

```

1:  $\epsilon$  = threshold value;
2:  $i = 1$ ;
3: while  $i \leq$  number of cell groups in  $H\_group$  do
4:   while there exists an unobserved pair of cells in  $H\_group(i)$  do
5:      $c_1, c_2$  = pair of cells in  $H\_group(i)$  that has not been observed;
6:     if  $M_{zz}(c_1, c_2) > \epsilon$ ;
7:       place cells  $c_1, c_2$  in  $cell\_group(i)$ ;
8:     end if
9:   end while
10:   $i++$ ;
11: end while
12:  $H\_group = cell\_group$ ;
13: return  $H\_group$ ;
```

Fig. 4. Pseudo-code for grouping together cells with high correlations.

IV. EXPERIMENTAL RESULTS

The majority gate, wire, and full adder were simulated using our proposed algorithm. The layout of the full adder is shown in Fig. 5. Based on the layouts of the simulated circuits, our algorithm grouped cells 4, 5, 6, and 10 together for the majority gate, and cells 7 and 8 for the long wire as shown in Fig. 6. The cell groupings for the full adder are shown in Fig. 6(c). In all cases, each circuit was simulated by modeling each of its cells as a 2x2 Hamiltonian and coupling them classically through expectation values (Hartree-Fock method). The grouped cells, which are enclosed in the

boxes, were modeled using separate Hamiltonians (a 16x16 Hamiltonian for the majority gate, for example), and then coupled classically to the rest of the system. The majority gate was simulated using the input pattern, 110, for inputs P_{driver1} , P_{driver2} and P_{driver3} , respectively, while the lone input for the wire was a logic 0. The full adder was simulated using inputs, $ABC_{\text{in}} = 001$. The results are shown in Figs. 7-9. In each case, using a threshold value, $\delta = E_k^0/10$, our algorithm was able to correctly settle to the correct ground state when the Hartree-Fock approximation failed to do so.

Further refinement was achieved for the majority gate, reducing the number of grouped cells such that it only included cells 4 and 5. Further refinement was also achieved for the full adder. In both cases, the reduced Hamiltonian model was able to correctly find the ground state.

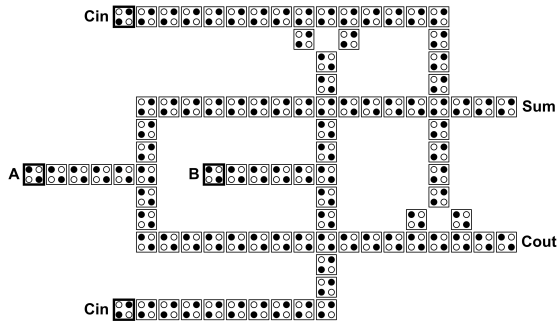


Fig. 5. Layout of the QCA full adder with no crossover.

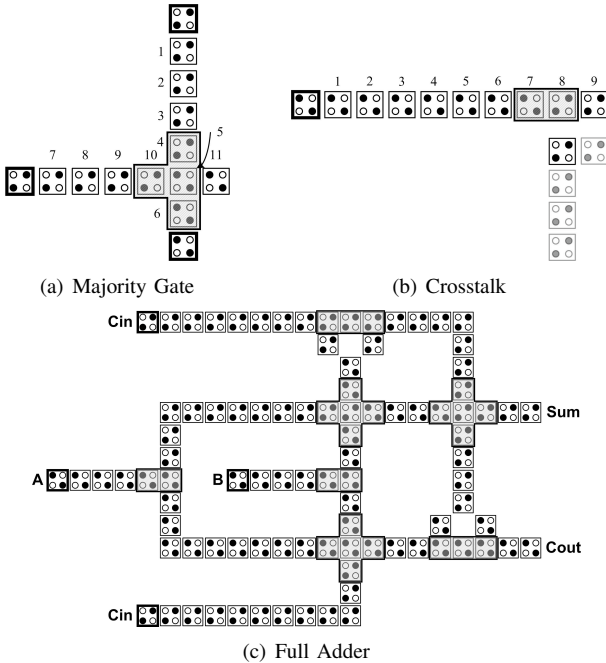


Fig. 6. Cells modeled using a multi-cell Hamiltonian.

V. CONCLUSIONS

An algorithm to determine *a priori* the highly correlated areas of a QCA circuit is presented in this paper. The inter-cellular Hartree-Fock approximation, which neglects quantum

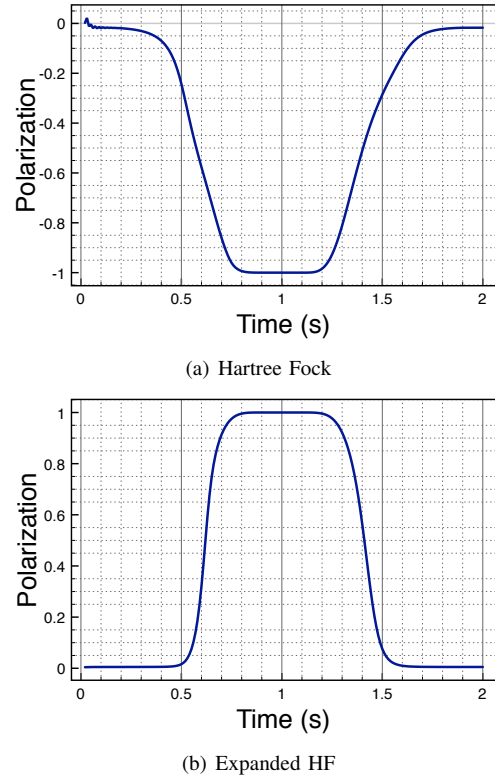
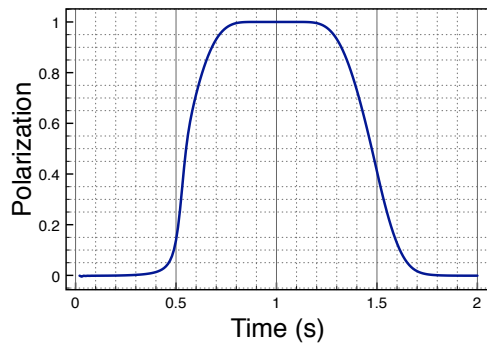


Fig. 7. Results for the majority gate using the Hartree-Fock and the Expanded Hartree-Fock methods.

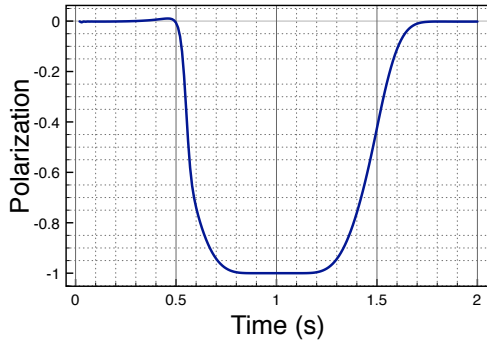
correlations between neighboring cells, is modified such that highly correlated groups of cells in a QCA circuit are modeled using a separate Hamiltonian and then coupled classically to the rest of the system. A refinement algorithm which attempts to reduce the size of these Hamiltonians using two-point correlations is also described in this work. Simulation results show that our algorithm can correctly find the ground state of common QCA building blocks such as the majority gate and wire, as well as the QCA full adder - all of which have shown to settle to meta-stable ground states when using the Hartree-Fock approximation.

REFERENCES

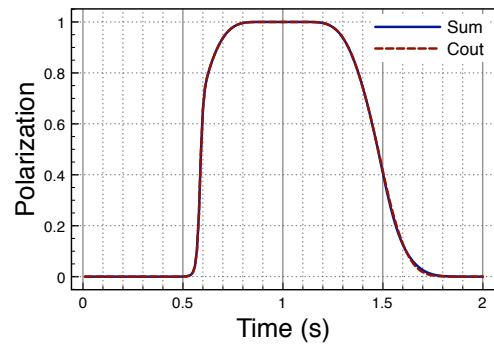
- [1] C. S. Lent, "Quantum cellular automata," *Nanotechnology*, vol. 4, pp. 49–57, 1993.
- [2] M. Macucci, M. Gattobigio, L. Bonci, G. Iannaccone, F. E. Prins, C. Single, G. Wetekam, and D. P. Kern, "A qca cell in silicon-on-insulator technology: theory and experiment," *Superlattices Microstruct.*, vol. 34, pp. 205–211, September 2004.
- [3] A. O. Orlov, R. K. Kumamuru, R. Ramasubramaniam, C. S. Lent, G. H. Bernstein, and G. L. Snider, "Clocked quantum-dot cellular automata shift register," *Surf. Sci.*, vol. 532–535, pp. 1193–1198, 2003.
- [4] I. Amlani, A. O. Orlov, G. Toth, G. H. Bernstein, C. S. Lent, and G. L. Snider, "Digital logic gate using quantum-dot cellular automata," *Science*, vol. 284, pp. 289–291, April 1999.
- [5] I. Amlani, A. Orlov, G.L. Snider, and C.S. Lent, "Demonstration of a functional quantum-dot cellular automata cell," *J. Vac. Sci. Technol. B*, vol. 16, pp. 3795–3799, 1998.
- [6] C.S. Lent, G.L. Snider, G.H. Bernstein, W. Porod, A. Orlov, M. Lieberman, T. Fehlner, M.T. Niemier, and P. Kogge, *Quantum-Dot Cellular Automata*. Boca Raton, FL, USA: Kluwer Academic Publishers, 2003.
- [7] G.L. Snider, I. Amlani, A. Orlov, G. Toth, G. Bernstein, C.S. Lent, J.L. Merz, and W. Porod, "Quantum-dot cellular automata: Line and majority gate logic," *Jpn. J. of Applied Physics*, vol. 38, pp. 7227–7229, 1999.



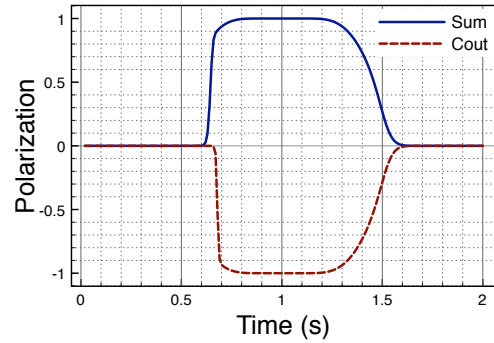
(a) Hartree Fock



(b) Expanded HF



(a) Hartree Fock



(b) Expanded HF

Fig. 8. Results for the wire using the Hartree-Fock and the Expanded Hartree-Fock methods.

Fig. 9. Results for the full adder using the Hartree-Fock and the Expanded Hartree-Fock methods.

- [8] R.V. Kumamuru, J. Timler, G. Toth, C. S. Lent, R. Ramasubramaniam, A. Orlov, and G.H. Bernstein, "Power gain and dissipation in a quantum-dot cellular automata latch," *Appl. Phys. Letters*, vol. 81, pp. 1332–1334, 2002.
- [9] G. Toth and C. S. Lent, "Quasiadiabatic switching of metal-island quantum-dot cellular automata," *J. Appl. Phys.*, vol. 85, no. 5, pp. 2977–2984, 1999.
- [10] Imre, A. and Csaba, G. and Ji, L. and Orlov, A. and Bernstein, G. H. and Porod, W., "Majority Logic Gate for Magnetic Quantum-Dot Cellular Automata," *Science*, vol. 311, no. 5758, pp. 205–208, 2006.
- [11] C. G. *et al.*, "Nanocomputing by field-coupled nanomagnets," *IEEE Trans. Nano.*, vol. 1, no. 4, pp. 209–213, 2002.
- [12] C. György and W. Porod, "Simulation of field coupled computing architectures based on magnetic dot arrays," *J. Comp. Elec.*, vol. 1, no. 1, pp. 87–91, 2002.
- [13] M. C. B. Parish, *Modeling of Physical Constraints on Bistable Magnetic Quantum Cellular Automata*. PhD thesis, University of London, 2003.
- [14] M. E. W. R. P. Cowburn, "Room temperature magnetic quantum cellular automata," *Science*, vol. 287, pp. 1466–1468, 2000.
- [15] G.H. Bernstein, A. Imre, V. Metlushko, L. Ji, A. Orlov, G. Csaba, and W. Porod, "Magnetic QCA Systems," *Microelectronics Journal*, vol. 36, pp. 619–624, 2005.
- [16] Y. Lu and C. S. Lent, "Theoretical Study of Molecular Quantum-dot Cellular Automata," *J. Comput. Elec.*, vol. 4, pp. 115–118, 2005.
- [17] C. S. Lent, B. Isaksen, and M. Lieberman, "Molecular quantum-dot cellular automata," *J. Am. Chem. Soc.*, vol. 125, pp. 1056–1063, 2003.
- [18] J. Jiao, G. J. Long, F. Grandjean, A. M. Beatty, and T. P. Fehlner, "Building blocks for the molecular expression of quantum cellular automata. isolation and characterization of a covalently bonded square array of two ferrocenium and two ferrocene complexes," *J. Am. Chem. Soc.*, vol. 125, no. 25, pp. 7522–7523, 2003.
- [19] C. S. Lent and B. Isaksen, "Clocked molecular quantum-dot cellular automata," *IEEE Trans. Electron Devices*, vol. 50, no. 9, pp. 1890–1896, 2003.
- [20] Z. Li and T. P. Fehlner, "Molecular qca cells. 2. characterization of an unsymmetrical dinuclear mixed-valence complex bound to a au surface by an organic linker," *Inorg. Chem.*, vol. 42, no. 18, pp. 5715–5721, 2003.
- [21] Z. Li, A. M. Beatty, and T. P. Fehlner, "Molecular qca cells. 1. structure and functionalization of an unsymmetrical dinuclear mixed-valence complex for surface binding," *Inorg. Chem.*, vol. 42, no. 18, pp. 5707–5714, 2003.
- [22] Qi, H., Sharma, S., Li, Z., Snider, G.L., Orlov, A.O., Lent, C.S., and Fehlner, T.P., "Molecular quantum cellular automata cells. electric field driven switching of a silicon surface bound array of vertically oriented two-dot molecular quantum cellular automata," *J. Am. Chem. Soc.*, vol. 125, no. 49, pp. 15250–15259, 2003.
- [23] K. Walus and G. A. Jullien, "Design tools for an emerging soc technology: quantum-dot cellular automata," *Proc. IEEE*, vol. 94, pp. 1225–1244, June 2006.
- [24] K. Walus, T. Dysart, G. A. Jullien, and R. A. Budiman, "QCADesigner: A rapid design and simulation tool for quantum-dot cellular automata," *IEEE Trans. Nano.*, vol. 3, pp. 26–31, March 2004.
- [25] K. Walus, R. A. Budiman, and G. A. Jullien, "Split current quantum dot cellular automata - modeling and simulation," *IEEE Trans. Nano.*, vol. 3, pp. 249–255, June 2004.
- [26] K. Walus and G. Schulhof, "QCADesigner Homepage," [Online] <http://www.qcadesigner.ca/>, 2001.
- [27] K. Walus, M. Mazur, G. Schulhof, and G. A. Jullien, "Simple 4-bit processor based on quantum-dot cellular automata (QCA)," in *Proc. of Application Specific Architectures, and Processors Conference*, pp. 288–293, July 2005.
- [28] K. Walus, G. Schulhof, R. Zhang, W. Wang, and G. A. Jullien, "Circuit design based on majority gates for applications with quantum-dot cellular automata," in *Proc. of IEEE Asilomar Conference on Signals, Systems, and Computers*, November 2004.
- [29] K. Walus, G. Schulhof, and G. A. Jullien, "High level exploration of quantum-dot cellular automata (QCA)," in *Proc. of IEEE Asilomar Conference on Signals, Systems, and Computers*, November 2004.
- [30] G. Toth, *Correlation and Coherence in Quantum-Dot Cellular Automata*. Ph.d., University of Notre Dame, 2000.
- [31] G. Tóth and C. S. Lent, "Role of correlation in the operation of quantum-dot cellular automata," *J. Appl. Phys.*, vol. 89, pp. 7943–7953, June 2001.