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Rules for a Cellular Automaton to Model Quantum-Dot Cellular Automata

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Abstract

Quantum-dot cellular automata are one of several new device architectures whose operation is based on local interactions, much like cellular automata. We have implemented several rule sets for a cellular automaton that could be used to model the behavior of quantum-dot cellular automata and used them to test most of the wire and gate configurations proposed for these devices. Arrangements of cells for which any particular cell has neighbors which are not adjacent to each other generally behave as expected. Unfavorable arrangements of cells such as those with bends and crosses tend to either have incorrect outputs or be unstable for some of the possible inputs. These results suggest that quantum-dot cellular automata need more than strictly local interactions in order to operate correctly.

1. Introduction

Much of the improvement in performance of large-scale integrated circuits over the years has been achieved by reducing the size and thus increasing the density of the component devices but this process is limited by a number of effects. As devices get more closely packed, the amount of heat generated gets so large that operating temperatures of the devices rise, degrading the performance of the devices. Also parasitic capacitance from the the necessary electrical connections between devices limits the speed of the devices. Finally, as devices sizes shrink, quantum mechanical effects are likely to dominate device behavior. New device designs will need to mitigate, or better yet, take advantage of these quantum effects.

Cellular automata (CA) are discrete dynamical systems whose evolution is based on local interactions. Bate [1] proposed the possibility of devices that operate like cellular automata in the sense that they interact via local forces instead of current-carrying wires. One particular device of this type which has been investigated in great

detail is quantum-dot cellular automaton (QCA) proposed by Lent *et al.* [2].

A QCA device typically consists of four quantum dots located on the corners of a square. These dots are populated by four electrons with a matching positive background charge to keep the device electrically neutral. The dots are located close enough together that electrons can tunnel between the dots. Coulomb interactions between the electrons are expected to constrain the system to two possible states. By combining a number of these devices, the functionality of conventional logic gates can be produced.

The possibility of creating the CA analogue of QCA has been suggested [2] but no published work on the subject has appeared. In this paper, we report our attempts to design a CA to model QCA. One reason for doing this is to determine whether such a CA is possible at all. If it is possible, the CA could be used for modeling QCA circuits.

2. Implementing the Cellular Automaton

A CA consists of a uniform cellular space which is defined by the allowed states for the cells, the neighborhood of the cells and a set of transition rules. Each cell can exist in any of a finite number of states. The neighborhood of a cell consists of the cells with which it interacts. The final component of a CA is the transition rules which determine how the states of the cells change with time. The following paragraphs describe our implementation of each of these components.

There are two electrons and four dots in a QCA cell. Classically, each electron could go into any of the dots but under most circumstances, the Coulomb repulsion between the electrons should insure that the two electrons will occupy diagonally opposite positions. For the purposes of this work, it will be assumed that only these two states will occur. Thus, a CA that models the idealized QCA system being explored here needs to provide for cells of two polarities. These will

Table 1: States needed for a CA to represent QCA.

State	Cell Type	Polarization	Status
0	quiescent cell	0	fixed
1	input cell	1	fixed
	control cell	1	fixed
2	input cell	-1	fixed
	control cell	-1	fixed
3	output cell	1	variable
	active cell	1	variable
4	output cell	0	variable
	active cell	0	variable
5	output cell	-1	variable
	active cell	-1	variable

be designated +1 which corresponds to logical 1 and -1 for logical 0. An unpolarized cell with the electrons uniformly distributed is also possible; this will be designated state 0. The circuits that are built with QCA do not have devices located at every possible location, so the CA also needs to have a null state to represent cells which do not contain devices. For input cells and for the control cell of a majority gate, cells which are fixed in a particular state are needed.

The states used in the work described here are summarized in Table 1. State 4 represents unpolarized cells which either haven't yet been assigned a state or have a symmetric neighborhood. State 0 is used for lattice positions which don't contain a QCA device. A QCA circuit has devices at fixed positions; they cannot appear and disappear as a function of time. Because the QCA are intended to be used in circuits or computations, it is convenient to have cells that are designated input and output cells but these are not functionally distinct states.

Because the behavior of some of the gates described for QCA depend on diagonal interactions, a neighborhood of at least 8 cells is needed for the CA. Since the Coulomb interaction is long-range, larger neighborhoods may be needed to accurately reflect the physical processes that occur in QCA systems. Tougaw and Lent [3] suggest that interactions are likely to occur over three intercellular distances. For this work, the neighborhoods explored include a maximum of 24 cells which corresponds to two intercellular distances. Adding more cells to the neighborhood would be straightforward but unlikely to significantly change the conclusions of this study.

Some care has to be taken in laying out circuits for testing so that circuit elements that are meant to be independent are far enough away from each other that cells in one aren't within the neighborhood of the cells in the other. Presumably, some such design rules would also be needed in real QCA circuits.

Three sets of transition rules were investigated. The first sets of rules are based on majority voting; each neighbor casts a vote to determine the next state of a cell. The simplest way to do this is to give all neighbors an equal vote. The state of a cell in the next cycle is determined by the sign of the sum of the votes of all its neighbors. Horizontal and vertical neighbors have a vote of 1 since such cells tend to have the same polarization. Neighbors located on the diagonal have a vote of -1 to reflect the fact that QCA cells located diagonally tend to alternate polarity. For the larger neighborhood, there are four cells in the outer ring which are situated symmetrically enough relative to the center cell that they are given no vote in the outcome.

Because the Coulomb effect is inversely proportional to distance, it is physically unreasonable to expect the magnitude of the effect of all neighbors to be the same. To empirically correct for this effect, a set of weighted voting rules was developed. The center-to-center distance between two diagonal cells is $\sqrt{2}$ times that of lateral neighbors. To approximate this, diagonal neighbors were given a vote with magnitude $\frac{2}{3}$ that of the lateral ones in the same ring. Neighbors in the second ring were given a weight that is half that of those in the first ring since they are twice as far away on average. These weights are

-2	0	3	0	-2
0	-4	6	-4	0
3	6	6	6	3
0	-4	3	-4	0
-2	0	6	0	-2

Figure 1: Voting weights of the neighboring cells for weighted voting rules.

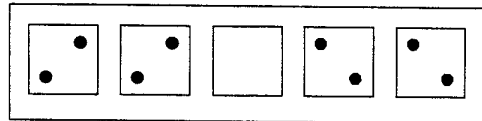


Figure 2: A symmetric configuration of cells that results in an unpolarized cell.

shown in Figure 1.

It is possible to have symmetric configurations of neighbors which result in a net vote of zero. An example of such a situation is shown in Figure 2. Under these circumstances, some kind of tie-breaking is needed if cells are required to be in one polarization or the other as might be expected physically. Three different approaches were implemented. In the first approach, cells were allowed to be in a neutral state. The second approach was to leave the cell in the same state it was in to begin with. This has the effect of giving the cell a vote in its future. The third approach was random tie-breaking. In a sense, this method reflects the fact that not everything in a real device can be completely controlled; there are always some random effects present.

The final technique for determining how a cell should change in response to its neighbors is to determine which polarity results in the lowest energy. The total Coulomb energy of each

$$W_{Coulomb} = \sum_{j=1}^m \sum_{k=j+1}^m \frac{q_1 q_2}{4\pi\epsilon r_{jk}} \quad (1)$$

possible configuration is calculated for both polarities of the central cell. A cell will take the polarity which results in the lowest energy. If both polarities have equal energy, the cell will be given a polarity of 0. Tie-breaking is used to resolve this as it was for the voting rules.

3. Results

Most of the wire and gate configurations proposed for QCA have been tested using the rules discussed above. The results for wires will be discussed in detail and the results for the gates will be summarized. More detailed results can be found in Cole [4].

Figure 3a shows the progression of changes for a wire consisting of a line of cells of which only the input cell is initially polarized. The polarization of the input cell propagates down the wire as the CA runs. The final state of the wire is the correct one independent of both the rules used for the CA and the size of the neighborhood. The propagation of an input polarization down an initially quiescent diagonal wire works as expected for neighborhoods consisting of 8 cells. For a 24-cell neighborhood, however, the signal doesn't propagate properly as can be seen in Figure 3b. Initially, the input cell switches the next two cells down the line, into the same polarity creating a *kink*. Once this kink forms, it tends to persist. Ultimately, the wire oscillates between two states with outputs of opposite polarity. Effectively, the update scheme for the CA prevents the system from correcting itself.

Initial configurations in which all the cells are initially polarized do not work as well. Figure 4a shows a starting configuration in which all cells but the input cell take the final polarizations of

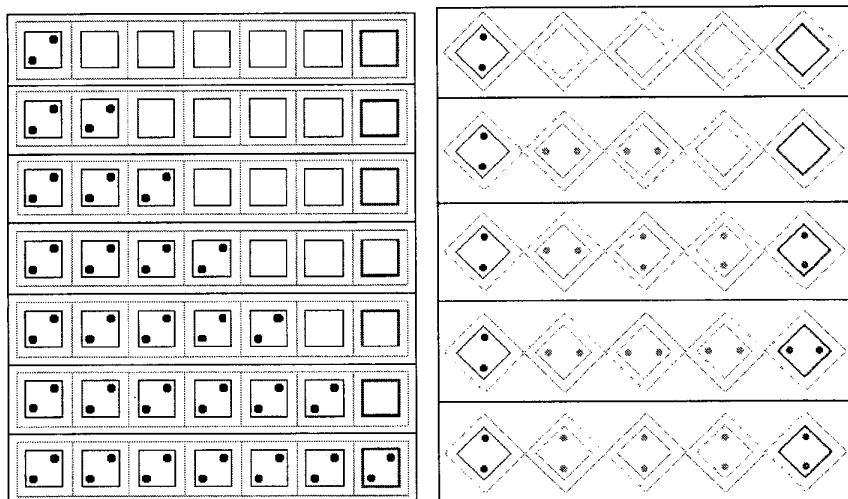


Figure 3: Stages in the CA operation of initially quiescent wires. a) Regular wire. b) Diagonal wire.

a wire that has a particular input and the polarization of the input cell is switched. If the CA is allowed to run from this initial state, it does not switch properly. If there is no tie-breaking, the cell next to the input becomes unpolarized and does not change further as shown in Figure 4b. If the current state is used to break the tie, the wire remains in the initial configuration indefinitely. This is also true if the neighborhood is made larger. The only case in which the CA gives the proper results for this initial state is the case of an 8-cell neighborhood with random tie-breaking. Here the output will eventually settle to the desired state but not very efficiently. The 7-cell wire of figure 4a was run 1000 times with an 8-cell neighborhood and random tie-breaking. The average number of cycles needed to reach the final configuration was 52 compared to the 6 cycles needed in the ideal case. Similar behavior is observed for a diagonal wire which has been initialized in the same way. With 24 neighbors, even random tie-breaking is not enough to allow the wires to reach the desired final state.

A wire with a bend also leads to problems. A progression similar to that in the previous figure is shown in Figure 5. The problem can be seen by looking at the second and third parts of the figure. The cell before the corner will cause both the corner cell and the first cell around the corner to switch. However, these two cells switch to opposite polarities. The corner cell is now in a symmetric neighborhood; with no tie-breaking,

it will become unpolarized in the next cycle. The circuit as a whole oscillates between two final states. Using the current state to break the tie also results in a cyclic final state. The last two cells remain perpetually out of phase with each other. Using a larger neighborhood results in a stable but incorrect final state. A bent diagonal wire has basically the same behavior as a straight one.

4. Summary

Several possible sets of CA rules that could be used to represent the operation of QCA have been investigated. Both empirical rules that implement the qualitative arguments that are useful for describing QCA operation and rules determined from a classical calculation of the Coulomb energy for each possible configuration have been investigated. Interaction over one and two intercellular distances have been investigated. Most of the wire and gate configurations that have been suggested for QCA were tested using these rules. The overall behavior of the CA did not vary significantly between the different combinations of options studied. Some general observations about the CA behavior are discussed below.

In general, the CA worked well only for configurations which satisfy some fairly restrictive layout guidelines. Arrangements of cells which are

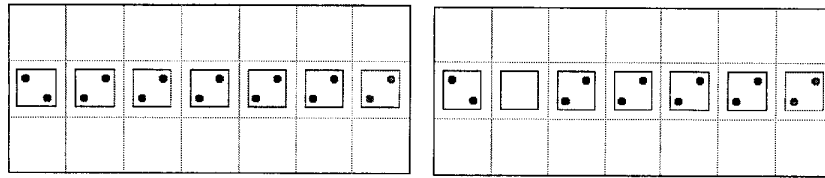


Figure 4: Stages in the CA operation for a regular wire whose input has been switched from one polarization to the opposite. a) Wire after input has been switched. b) After one cycle with no tie-breaking.

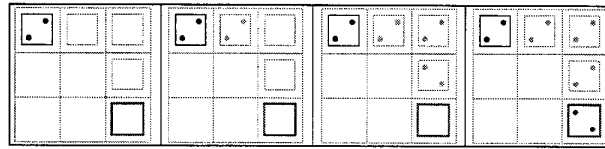


Figure 5: Stages in the CA operation for an initially quiescent wire with a bend in it.

relatively sparse generally behave as desired for most of the rule sets that were tested. Sparseness is not an absolute measure but depends on the relative positions of cells. Arrangements of cells for which any particular cell has neighbors which are not adjacent to each other are considered to be sparse. Unfavorable arrangements such as those with bends and crosses tend to either have incorrect outputs or be unstable (oscillatory) for some of the possible inputs. Any configuration which has one or more cells with neighbors that are adjacent to each other is likely to result in “conflicted” configurations, that is situations where the active cell and one of its neighbors are trying to force their common neighbors into opposite polarities. This commonly results in cyclic behavior but can also result in incorrect logic. The fact that several neighbors get switched at the same time suggests that trying to implement some kind of time-based tie-breaking would not be trivial. These results suggest that QCA based on Coulomb effects will need something other than strictly local interactions if they are to operate correctly.

For all of the circuit elements tested, the desired final state of the circuit was stable. The problem is that this stable state isn’t necessarily reached from the initial configurations that are likely to be encountered. Switching an input from one polarity to the other generally results in a logically incorrect state for the CA. In some measure, this is related to the problem of tie-breaking discussed below. Another factor, is

that there can be a number of stable final configurations for a particular choice of inputs in a given circuit. For many circuit elements and probably for most circuits combining these elements, there can be a number of stable and cyclic configurations which have the same configuration of input cells. This is clearly not a desirable situation for computation.

QCA are supposed to compute the result of a calculation by finding the ground state (minimum energy state) of an arrangement of cells that represents the problem to be solved. The CA designed here, particularly the one in which the rules are based on calculations of the Coulomb energy of the cells in a neighborhood, minimizes the energy within each neighborhood separately. This is not necessarily the same as minimizing the total energy since the total energy of the system includes terms that aren’t included in any of the local energy calculations.

Symmetric neighborhoods appear rather frequently in the CA even though the circuit as a whole is not at all symmetric. This suggests that adiabatic switching [5] is likely to be necessary to the successful implementation of QCA. An effective tie-breaking mode is difficult to implement. Any deterministic method of selecting the polarization of the affected cell is likely to be wrong some of the time. Using a random assignment provides the most opportunity for the CA to evolve away from an incorrect logical state but there is no guarantee that this will happen

in a timely manner. In the worst case, it could take an arbitrarily long time.

There are a number of ways that the current work could be extended in addition to the trivial extension to larger neighborhoods. Other approaches to tie-breaking, such as one that gives a larger vote to cells which have changed most recently could be implemented. Asymmetric rules that distinguish between input and output in some way could be explored. A CA that has states and rules corresponding to the rotated cells that allow for wire crossing would make it possible to test more interesting circuits. A 3-dimensional CA could be devised to investigate whether layering improves the CA operation. Another improvement that could be added to the enumerated rules is to allow for non-logical states of the QCA cell.

The results of this study suggest that designing a CA that accurately models ideal QCA behavior is difficult. The following argument suggests that the existence of a CA that accurately models QCA is improbable. If QCA truly behave as advertised, then it ought to be possible to solve boolean satisfiability by building the circuit of interest and running it backwards. If the QCA settles to a logically correct ground state, which can easily be checked, then the circuit is known to be satisfiable. If this happens in a polynomial amount of time, then according to Lusth and Dixon [6], $P = NP$. If $P \neq NP$, as many people believe, it would be impossible to create a CA that models QCA in polynomial time.

QCA cells have some interesting properties that make them worth studying as a computational paradigm. Up until now, work in this area has

focused on using these devices by replacing conventional elements in a circuit by their QCA analogs. This is straightforward but may not ultimately be the best approach. With a new computing paradigm, there might be new ways to implement the logic of computing as well. What is needed is a way to harness the power of computing via energy minimization. A CA is essentially a parallel device; a device architecture based on this paradigm should be able to do much more than perform serial computations.

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