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Short Communication

Eliminating non-logical states from linear quantum-dot-cellular automata

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Abstract

Quantum-dot-cellular automata are a method of computing with small numbers of electrons. The static shape of a particular automaton corresponds to a problem to be solved while the time-dependent evolution of the distribution of electrons within the automaton corresponds to a computation to solve the problem. The final distribution of electrons within the automaton represents a solution. The robustness of an automaton is characterized as the absolute energy difference between the lowest energy state and the first excited state. For computing IDENTITY, a basis for translating values across a larger system, it is shown that the robustness of the automaton can be improved dramatically by redesigning to eliminate non-logical states. By such redesign, the states that populate the energy levels between the logically correct answer and logically incorrect answers are prohibited, thereby increasing the energy gap between the ground state and the first excited state.

Keywords: Computer architecture; Quantum-dot-cellular automata

1. Introduction

Feature sizes in computer chip manufacturing are becoming so small that eventually the function of solid-state devices will be limited by quantum-mechanical effects. Accordingly, various proposals have been put forth to perform computations *using*, rather than *avoiding*, the quantum-mechanical behavior of a small number of electrons. In contrast to pure quantum computing, another avenue envisions computing devices composed of arrays of quantum wells, or dots, each of which can trap and hold a single electron [1–4]. The first detailed proposal concerning this approach came from Lent et al. [5], in which electrons populate specially constructed cellular arrays. They named their class of computing devices *quantum-dot-cellular automata* or QCA. In an automaton, the distribution of electrons in the lowest energy, or ground state encodes the result of a computation. Their ideas have garnered much attention because they seem to be physically realizable in the near term [6].

The viability of QCA hinges upon three assumptions: that individual QCA logic devices can be combined hierarchically [7,8] into a sort of quantum-cellular circuit, that an automaton can be driven into its lowest energy state without becoming stuck in local minima [9,10] and that QCA can compute at reasonable temperatures. With regards to the third assumption, Lent and Tougaw [9] claim that QCA can compute below 7 K.

Such a low operating temperature is necessary to distinguish the ground (lowest energy) state from the first excited (next higher energy) state. More precisely, QCA will correctly resolve to the ground state if the *viability relation*, $((kT)/\Delta)\ \ln(n) < 1$, holds, where k is Boltzman's constant, T is temperature, Δ is the energy difference between the two lowest energy states, and n is the number of cells in the automaton [9]. In this paper, it is shown that first excited states for some simple problems are composed of cells with *non-logical* interpretations. If these states can be prohibited, then Δ, the gap between the ground state and the next higher energy state, increases. Consequently, the temperature at which these automaton will function correctly will increase. In the next section, a description of how QCA operate is given along with a definition of the term *non-logical*.

2. Background

QCA are composed of arrays of identical cells, with each cell containing four quantum wells, or dots. Each cell contains two electrons, which are allowed to tunnel between dots, but are not allowed to leave the cell. Although QCA cells switch states internally via quantum-mechanical tunneling of electrons between quantum dots, the electronic

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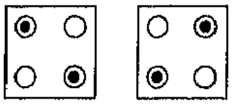

Fig. 1. A basic quantum cell and its two orientations (zero on the left, one on the right) when populated with two electrons.

configuration of a QCA array is determined by the classical Coulombic repulsion between electrical charges. Because the two electrons tend to repel each other, there are two preferred orientations for the cell, suggesting a binary signal. Fig. 1 shows the two preferred orientations, which have maximal separation between the two electrons inside a cell.

By convention, the orientation of the leftmost cell in Fig. 1 is considered a logical zero, while the orientation of the rightmost cell in the figure is considered a logical one. Due to the Coulomb interaction, the orientation of a cell influences the orientations of its neighbors. Thus, each cell affects every other cell in an automaton, either directly or indirectly. To begin a computation, the input is represented as a bitstring, and the orientations of a set of input cells are fixed to represent the input. The automaton is then allowed to relax to the ground state. At this point, the orientations of another set of cells, designated output cells, reflect the computational result, again encoded as a bitstring. Simple QCA exist for performing basic logical tasks, such as OR and NOT [8]. By combining these simpler QCA into more complex automata, it should be possible to compute any computable function via QCA.

A cell is considered to be in a *non-logical* state if the preferred classical distribution of its two electrons does not match either of the configurations shown in Fig. 1. In addition to the two logical distributions, there are four non-logical distributions corresponding to the electrons occupying wells on the same side of the cell. Finally, there are four additional non-logical states, wherein two electrons occupy a single dot.

We shall make use of a classical model in which the allowed electronic distributions are catalogued in Fig. 2. This classical model assumes that the tunneling energy for electrons is much smaller than the Coulomb energy gap

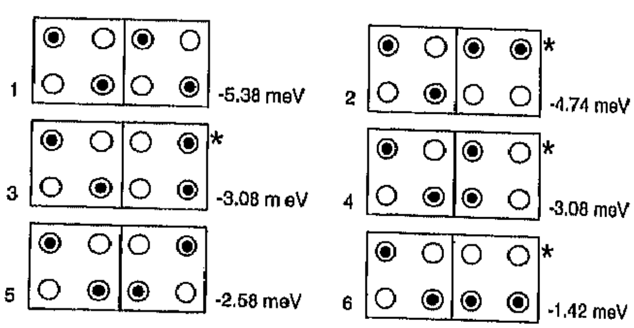

Fig. 2. A ranking of the energy states for the two-cell QCA for solving the identity function. Numbers to the right are rankings while numbers to the left give absolute energies. Asterisks mark the non-logical cells.

between the ground and the first excited states. We also assume that the energy for two electrons to occupy the same quantum dot is much higher than the energies of the configurations shown in Fig. 2. Results similar to those found in this paper would also follow from a quantum-mechanical treatment, in the limit of small inter-dot tunneling energies. For more justification on using a classical model, see Ref. [11].

The classical computation of energy proceeds by summing over all pairs of charges:

$$E = \frac{1}{2}\sum_{i \neq j} \frac{q_i q_j}{4\pi\varepsilon r_{ij}},$$

where q_i and q_j are the charges in the pair, ε is permittivity of the space separating the charges, and r_{ij} is the distance between the charges. We introduce compensating positive charges to provide for electrical neutrality for QCA cells. As in Ref. [12], the distribution of compensating charges is idealized; a charge of $+e/2$, where e is the charge of a proton, is assigned to each dot in the cell. Thus an occupied quantum dot is considered to have a charge of $-e/2$ while an unoccupied dot is considered to have a positive charge of $+e/2$. Girlanda et al. [13] present a more realistic treatment of compensating charges. The permittivity of QCA is taken to be $\varepsilon = \varepsilon_r\varepsilon_0$, where ε_r is the relative dielectric constant for the semiconductor medium of the QCA and ε_0 is the permittivity of free. We take $\varepsilon_r = 11.7$, corresponding to silicon.

3. QCA for computing identity

One of the simplest problems to solve is IDENTITY, a basis for a QCA wire [12] and useful for translating a particular value across the span of a larger automaton. Given two adjacent cells, if one cell is fixed logically to a zero or one (the input cell), will the adjoining cell (the output cell) reflect the same logical state as well? The answer is yes, but at the given dimensions of an intracellular dot-spacing of 20 nm and a intercellular spacing of 60 nm [12], Δ is a slim 0.16 meV. The first excited state has the adjoining cell in the logically opposing orientation. However, by changing the intracellular dot-spacing to 40 nm (essentially keeping within the same manufacturing tolerances — no two dots are closer than 20 nm), Δ increases to 0.64 meV, a four-fold improvement. Moreover, at these dimensions, non-logical states crop up between the logically correct and the logically incorrect state. Removal of these states will boost Δ further.

Fig. 2 gives a ranking of all the possible states of the two-cell automaton based upon a 40 nm intracellular dot-spacing and a 60 nm intercellular spacing. Note that, if the non-logical states 2, 3, and 4 could be excluded, Δ would improve to 2.8 meV, a 17-fold improvement.

The presence of non-logical states is a direct consequence of having more than two degrees of freedom for the electrons in a cell. If N is the number of quantum dots in a cell

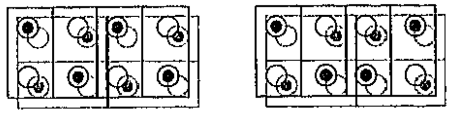

Fig. 3. The two lowest energy states in the two-layer system (ground state on the left).

and R is the number of electrons, then the constraint

$$\binom{N}{R} = 2$$

ensures that a cell can only exist in a logical state. Unfortunately, there is little choice in enforcing this constraint; it only holds if N is two and R is one. Still, one can envision the automaton shown in Fig. 2 as a series of two-dot cells by simply dividing each four-dot cell into two rows with one electron per row. As before, an electron may tunnel to the other dot in the row, but cannot leave the row. If this is done, then state 2 is prohibited, increasing Δ to 2.3 meV.

Is it then possible to eliminate the newly penultimate states 3 and 4? One could have prohibited them by dividing the four-dot cells into columns instead of rows, but then state 2 would be still be allowed. It is easy to see that with the types of cells described here, one cannot eliminate all three intervening non-logical states through such manipulations. There is, however, an engineering trick that can be used to get the best of both worlds and push the remaining non-logical states higher than the logically incorrect state 5.

Consider a four-cell automaton composed of two two-cell automata layered one directly above the other. The cells of the lower automaton are divided into two-dot rows while the cells of the upper automaton are divided into two-dot columns. In such a system, with a separation of 20 nm between layers (essentially maintaining the same manufacturing tolerances as before), the two states shown in Fig. 3 are the ultimate (left) and penultimate (right) energy states. Note that all cells have logical interpretations as desired. Δ is 3.0 meV, besting even the best possible result in the single-layer system. If the separation is widened slightly to 21.5 nm, Δ peaks at 3.2 meV, decreasing thereafter at wider separations. Is such a layered automaton feasible? Gin et al. [14] give an alternate geometry in which cells in a two-dimensional array are placed on edge in order to conserve die area. If one interprets top edges of such cells in isolation from the bottom edges, one sees a picture very much like that shown in Fig. 3. Thus, the two-layer system proposed herein should be as viable as that given in [14].

A QCA *wire* is the identity problem extended to an arbitrarily long chain of cells. In a wire, all other cells should reflect the state of the input cell. As more cells are added to the chain in the two-layer system described above, the same exclusion of non-logical states is seen. More importantly, Δ increases slightly and asymptotically. The same behavior is seen in the single-layer, two-dot cellular, system, although with an overall smaller Δ. In contrast, with the single-layer, four-dot cellular system, the Δ *decreases* asymptotically with increasing number of cells in the chain. Thus, the two-layer and single-layer, two-dot cellular chains offer a 14–20-fold increase in Δ over the originally proposed chains. The two-layer system has the added advantage that it functions correctly, regardless of whether the cells are chained from left-to-right or top-to-bottom (with respect to the page). The mono-layered two-dot cellular system needs to be row-ordered for left-to-right chains but column-ordered for top-to-bottom chains in order to provide the most useful elimination of non-logical states.

A note of caution is in order. Increasing the intracellular dot-spacing can be problematic because the probability for electrons to tunnel between quantum dots in a cell decreases exponentially with dot-spacing, if the energy barriers between the quantum dots are not reduced sufficiently. In a nice analysis of the limits of tunneling energy, Lent and Tougaw [4] found that for dot-spacings of up 40 nm, the cells in an automaton are still well polarized (the constants have yet to be overwhelmed by the exponential). Thus, the use of a 40 nm dot-spacing to increase Δ is justified.

4. Conclusions

The performance QCA for computing IDENTITY can be improved by outlawing non-logical states. The absence of such states increases the energy gap Δ between the ground state and the first excited state in many instances. With increased Δ, an automaton becomes more robust, allowing it to operate at higher temperatures. One method for eliminating non-logical states is to split the QCA cells into two compartments. This prohibits some, but not all of the non-logical states. Another method that does effectively remove the remaining non-logical states is to use a two-layer system. All the cells in a given layer are divided into two compartments in the same fashion, either by rows or by columns. In the opposing layer, cells are divided in the opposite fashion. This arrangement forces linear automata with non-logical cells to higher energy levels, leaving no states intervening between the desired ground state and the logically incorrect state. As hoped for, Δ in this system shows a roughly 20-fold increase over the originally proposed system. Using the viability relation of Section 2, this improvement should allow for operation of IDENTITY QCA at much higher temperatures, even when taking account of the increase in the number of cells, the quantum-mechanical effects, and a more realistic treatment of compensating charges.

Acknowledgements

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