The Development of Quantum-Dot Cellular Automata

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Abstract. Quantum-dot cellular automata (QCA) is a paradigm for connecting nanoscale bistable devices to accomplish general-purpose computation. The idea has its origins in the technology of quantum dots, Coulomb blockade, and Landauer's observations on digital devices and energy dissipation. We examine the early development of this paradigm and its various implementations.

Keywords: Quantum-dot cellular automata (QCA) · Molecular electronics

1 Introduction

Quantum-dot cellular automata (QCA) is a means of representing binary information in cells, through which no current flows, and achieving device performance by the coupling of those cells through the electromagnetic field. Information is stored in the arrangement of charge (or magnetic dipoles) with in the cell. Importantly, cells have no monopole moment and are designed to be bistable, having two low energy states with different dipole or quadrupole orientation which can encode a binary 1 or 0. For large scale structures it is necessary to guide the switching of the cells with a clocking field that controllably switches the cells between a null state and an active state (either 0 or 1). Clocking provides power gain necessary to restore signal energies which would otherwise decay due to inelastic losses. The interaction energy between two cell, that is the energy difference between neighboring cells holding the same or opposite bits, is termed the kink energy, and determines thermal stability. Raising the kink energy entails moving to smaller geometries, with molecular QCA providing the limit of device density and requiring the ultra-low power dissipation made possible by adiabatic switching of QCA.

Here we sketch the origins of the QCA idea, its early development, and subsequent evolution into several implementations and many research fronts. This is in no way a comprehensive review, but is particularly focused on the perspective of the Notre Dame group which originated the idea, and the basic trajectories that have arisen from the early work. We mean no slight by mentioning only a few of the major subsequent investigators. The elaboration of all the other contributors to this volume is necessary to give a fuller picture.

N.G. Anderson and S. Bhanja (Eds.): Field-Coupled Nanocomputing, LNCS 8280, pp. 3–20, 2014.
DOI: 10.1007/978-3-662-43722-3_1,

2 Historical Background

In the 1980's advanced epitaxial growth techniques such as molecular beam epitaxy (MBE) enabled the creation of GaAs-AlGaAs semiconductor heterostructures with very smooth interfaces. This ability to control the composition of crystalline semiconductors with atomic precision made possible the formation of a highly conducting two-dimensional electron gas (2DEG) at the interface between AlGaAs and GaAs. Moreover, the 2DEG, which was essentially a plane of confined electrons, could be further patterned by placing lithographically-defined metal gates on the surface of the semiconductor. A negative potential on the gates would deplete the 2DEG under the gate regions. In 1988 two groups measured quantized conductance through a constriction connecting two 2DEG regions and found that it was quantized [1, 2]. This was convincingly explained by invoking the quantum-mechanical nature of the electrons transiting the constriction. Using the effective mass approximation, one could explain much of the behavior of this layer by solving the Schrödinger equation in two dimensions.

The ability to engineer the effective wavefunction of electrons seemed very promising for potential device applications. Throughout the 1990's (and beyond) many wave-based device designs were proposed which used quantum interference effects as their operating principle, often created in analogy with microwave devices. Truly remarkable experimental demonstrations left little doubt that these quantum mechanical effects were real and could be potentially exploited for device behavior. In addition, it proved possible to create quantum dots by confining the 2DEG in both lateral dimensions (the third dimension was already confined by the heterostructure potential. These quantum dots could be viewed as artificial atoms [3, 4], and also as high-Q resonators for ballistic electron transport [5].

Into the optimism that these new abilities engendered, Rolf Landauer injected a ray of pessimism and realism. In a talk at the first International Symposium on Nanostructure Physics and Fabrication in 1991, Landauer cautioned that interference devices were unlikely to make it in the real world [6]. A "rich" response with many peaks and valleys did not, he argued, make a robust basis for devices, which would have to be tolerant of fabrication variations and environmental perturbations. He argued for devices whose transfer function is nonlinear and saturates at two distinct levels, as does a CMOS inverter. This input signal should be of the same type as the output signal, so that information can be transferred from device to devices.

Another stream of research at the time was the newly emerging and promising phenomenon of Coulomb blockade in small structures. Electrons tunneling onto small metal islands can raise the potential of the island by e2/C, where C is the total capacitance of the island [7]. For very small structures this charging energy could be significant compared to thermal energies. The "orthodox" theories of the Coulomb blockade, even when treating the system quantum mechanically, characterized the island by this macroscopic quantity—the capacitance [8]. While this is quite adequate for metal structures containing very many free electrons, in small semiconductors one should really use a multi-particle approach. In such a model the effective capacitance is a result of the calculation of Coulomb effects, rather than being an input to it.

A study of few-electron systems under bias showed a threshold behavior for single electron transfer that is very nonlinear [9]. The origin of this nonlinearity is fundamentally the quantization of charge. If a region of space is surrounded by barriers that are appropriately high, but still possibly leaky, then the expectation value of the enclosed charge will be very close to an integer multiple of the fundamental charge. When the equilibrium value of the charge changes because of a tunneling event, it will necessarily be a rather abrupt jump between two integers.

Finally, the QCA architecture was inspired by classical cellular automata (CA) architectures [10], of the type popularized by Conway's Game of Life. These are mathematical models of evolution that proceed from discrete generation to generation according to specified rules. The state of each cell is determined by the state of the neighboring cells in a previous generation. The neighbor-to-neighbor coupling is a natural match for nano-devices, since one expects that one very small device may influence its neighbors, but not distant devices. CA's represent a means of computation that departs from the current-switch paradigm of transistors. But cellular automata are mathematical models that can operate with any set of evolution rules. The question for device architecture was not simply what local CA rules will produce computational behavior, but what rules does the actual physics of cellular interaction support.

The original QCA idea was the result of the confluence of these four ideas: (1) the ability to create configurations of quantum dots which localize charge, (2) the convincing argument by Landauer that any practical device would need bistable saturation in the information transfer function, (3) the nonlinearity of charge tunneling between such dots because of charge quantization, and (4) the notion of a locally-coupled architecture in analogy to cellular automata.

It is worth noting that the connection to cellular automata is by analogy. Classical CA's are almost always regular one or two-dimensional arrays of cells. The physics of the interaction between QCA cells does not yield very interesting results for regular arrays. QCA circuits look more like wires connecting devices; highly non-regular layouts of cells provide the specific function. Mathematical model CA's evolve in discrete generations, but physical systems interact continuously.

3 Developments

The first QCA paper demonstrated the bistability of a QCA cell using a multi-electron Hamiltonian and a direct solution of the Schrödinger equation [11]. This direct approach avoided the problems of sorting out exchange and correlation effects; within the site model it was exact. This bistability remains a key feature of QCA. Though it is somewhat appealing to explore a multi-state QCA cell and multi-state logic, only a bistable system can truly saturate in both logic states. An intermediate state is always subject to drifting off from stage to stage.

It was soon realized that a line of QCA cells acted like a binary wire and a junction of two or three wires could form a logic gate [12]. The first proposal was to have a special cell at the junction which could be internally biased to the 1 or 0 state and thereby act as an OR gate or an AND gate [13]. It was soon clear that the bias could be

applied by another wire, forming a three-input majority gate [14]. Inverters could be formed from diagonal interactions between cells. With these basic elements, any logical or arithmetic function can be formed.

With a year of the first QCA publication, other implementations were suggested. Small metal islands could serve as dots and form QCA cells if they were coupled by tunnel junctions [15]. One advantage of metal-dot QCA is that the electric field lines from the dot can be guided by the conductors to influence the neighboring dots; in the semiconductor depletion dots, the field spreads out in all directions. It was also natural to envision molecular versions of QCA where the role of the quantum dot was played by a part of the molecule that could localize charge [14]. A magnetic model of QCA was constructed from three-inch magnets held in Lucite blocks which rotated on low-friction jeweled pivots. These magnetic cells were used during talks and lectures by both of the present authors to demonstrate QCA wires and gates. They prefigured (at enormous scale) the nanomagnetic QCA under active research today and discussed in other contributions to this volume.

A detailed examination of QCA dynamics and the development of several levels of quantum description of QCA arrays [16], were prompted by another observation of Landauer [17]. While encouraging QCA exploration, he expressed concern that a weak link in a QCA wire would cause a switching error because the incorrect "old" state downstream would have more influence than the upstream cells with the new state. By treating the whole wire quantum mechanically it could be shown that this would only be a temporary problem. But the exercise focused attention on the nature of computation in QCA systems, which were designed from the beginning to map the ground state onto the computationally correct state. This mapping can be robust, while the details of the transient response of the system are inherently more fragile. We wanted to avoid computing with the transient. A byproduct of these calculations was the development of several approximate treatments for both equilibrium and dynamic calculations. The mapping between QCA and the Ising model in a transverse field was also made precise.

Clocking of QCA arrays arose out of the detailed consideration of switching dynamics and the desire to retain the robustness of the mapping between the ground state and the computationally correct state for large systems. Clocking QCA entails gradually moving cells between a neutral state and an active state with a clocking signal. The active state can be either a binary 0 or 1; the neutral state is usually denoted as a "null" state that carries no information. The first version of clocking, proposed the year following the initial QCA papers, contemplated raising and lowering the inter-dot tunneling barriers [18, 19]. This would gradually (adiabatically) transition the cell between a delocalized electron configuration (null) and the localized configuration of the active state. Koroktov and Likharev subsequently suggested a version of metal-dot QCA called the single electron parametron which used a complicated rotating electric field as a clock [20]. This had several drawbacks (e.g., information could only move in one direction in an array), but the idea of using as the null state a localized state on an intermediate dot was adopted for clocking QCA, particularly for molecular implementations. It is much easier to change the potential on the intermediate dot than to directly influence the tunnel barriers between dots, and the effect is the same. Adiabatic clocking QCA [21] solved the problem of switching

dynamics getting caught, even temporarily, in a metastable state; this was the heart of Landauer's objection. It retained the advantages of (local) ground-state mapping. During switching each cell is always very close to its instantaneous ground state (the definition of adiabaticity). Though we did not fully appreciate it at the time, this essentially turned QCA into a concrete implementation of the gedanken experiments which had led Landauer to conclude that there was no fundamental lower bound to the energy that must be dissipated to compute a bit [22]. Clocking further allowed much larger computational structures to be envisioned, combining memory and processing.

3.1 Semiconductor QCA

The Cavendish group of Smith et al. demonstrated QCA operation in GaAs/AlGaAs heterostructures with confining top-gate electrodes [23–25], as originally envisioned in the earliest QCA publications. The group of Kern et al. demonstrated a QCA cell in silicon, using an etching technique to form the dots [26–29]. The group of Mitic et al. used a novel method to form dots from small clusters of phosphorus donors in silicon [30]. They succeeded in demonstrating QCA operation in that system. Interestingly, their long-term goal is coherent quantum computing and they conceive QCA devices as providing an ultra-low-power layer of interface electronics to connect a cryogenic quantum computer to standard CMOS electronics [31].

The challenges of all semiconductor implementations have been two-fold. Firstly, the lithographically accessible sizes for quantum dots are large enough that kink energies are low and cryogenic operation is required. More importantly, the perfection of the interface and electronic environment becomes an issue. While dots with tens of electrons effectively screen small amounts of impurity and imperfections, in the limit of single occupancy, semiconductor dots become very sensitive to the details of the environment. Even MBE-grown samples have enough random imperfections that the dot is often not exactly where one expects it to be based on lithography [32].

3.2 Metal-Dot QCA

Although electronic QCA has been demonstrated in a number of material systems, metal dot implementations have proven to be the most successful, so far, building on the fabrication techniques developed for single-electron transistors [33, 34]. The advantages of metal dots are that the fabrication yield is relatively high, and they are electrically well-behaved, meaning that energy required to add each additional electron to the dot typically remains constant over the addition of many electrons. This makes it easier to load the QCA cell with the proper number of electrons and to bias the cell so that the two polarizations are energetically degenerate. However, in semiconductor dots [33, 34] the fabrication yield is low and the addition energy typically differs for each additional electron, and the electrical behavior of the dot can change from run to run, making it difficult to prepare the cell for proper operation. This makes the metal dot an attractive option for QCA experiments. The main disadvantages of metal dots are background charge fluctuations [35], and low operating temperature. Background charge fluctuations are caused by the random arrangement

of stray charge in the vicinity of the QCA cell, which affects the bias point and polarization degeneracy of the cell. The arrangement of this charge changes with time, and the gate biases applied to each dot in the cell must be adjusted to keep the cell operational. The low operating temperature of metal dot QCA cell is due to the size of the lithographically defined cell.

The metal dot QCA are composed of aluminum islands separated by tunnel junctions. Fabrication of the cell is done by electron-beam lithography using the Dolan bridge technique [7] where the tunnel junctions are formed by evaporation of aluminum from two angles, with an intervening oxidation step. The resulting tunnel junctions are composed of two layers of aluminum separated by a thin layer, 1–2 nm, of aluminum oxide. The area of the overlap between the two layers of aluminum determines the capacitance of the junction, and since it is typically the dominant capacitance of the dot, determines the operating temperature of the QCA cell.

Cells and Logic

The first QCA cell was demonstrated in 1997 [36]. This device had a junction overlap area of approximately 50 × 50 nm, giving an operating temperature of 70 mK. As it was the first demonstration, the layout was very conservative and optimized for high yield, which resulted in a relatively large overlap and low operating temperature. In this first demonstration the goal was to use gate electrodes to move an electron between the top and bottom dots on the left side of a cell. The electron in the right half of the cell would move in the opposite direction to maintain the lowest energy configuration. To measure the polarization of the cell, single-electron transistors, which are the most sensitive electrometers demonstrated to date [37], are used to measure the potential of the dots in the right half of the cell. Measurements of the output of the two electrometers move in opposite directions, confirming that an electron in the right half moves in the opposite direction to the electron in the left half, confirming QCA operation. Full details of the experimental methods are given elsewhere [38–41].

The next step in the development of metal dot QCA was the demonstration of a logic gate [42]. The basic logic element in the QCA paradigm is the majority gate, where three inputs vote on the polarization of a QCA cell. For this experiment we again used metal dots defined by the Dolan bridge method. For the inputs of the majority gate we applied voltages to the input electrodes that mimicked the potentials of three input cells. The applied voltages were varied to step through the logic truth table. The polarization of the cell was measured by electrometers and the output of the cell confirmed proper operation of the gate.

These experiments showed the basic functionality of QCA cells. The next experiment [43] showed that a QCA line could switch without getting stuck in a metastable, partially switched, state. In this experiment three 2-dot cells were fabricated in a line, and an input applied to the left side of the line. Electrometers coupled to the output side of the line confirmed the proper switching.

Power Gain

These initial experiments used unclocked QCA cells, but clocking is an important element in QCA systems. Clocking of QCA cells is crucial to achieve perhaps the

most important quantity in a logic device: power gain. Without power gain the input signal would degrade in a line, due to the unavoidable energy dissipation at each stage, and fan-out would be impossible. Clocking in QCA requires a variable barrier to control the tunneling of electrons between dots. Since the tunnel barrier in metal dot QCA is a fixed aluminum oxide layer whose barrier height cannot be modulated, clocking dots are introduced into the QCA cell as intermediate dots. These dots are coupled to clock electrodes that control the potential of the central dots. A positive clock voltage pulls the electrons to the central dots to produce the null state. A negative voltage forces the electrons to leave in a direction that is determined by the cell's input. In the initial experiment, a differential input voltage is applied to the left side of the cell and electrometers measure the potential of the top and bottom dots of the right half of the cell. Measured output waveforms confirmed proper operation of the cell [44]. A clocked QCA cell can also be used as a latch, a short-term memory element, as demonstrated in our experiments [45, 46].

As shown by theory, the power gain of a QCA cell is not fixed. If the input is weak, the cell pulls power from the clock to restore the signal level. Since the signal energy is fixed for a given cell, the amount of power pulled from the clock will depend on the weakness of the input. An experimental demonstration of power gain involves a measurement of the charge on the dots of the QCA cell [43] as the inputs and clock are moved through one clock period. In this way the work done by the input on the cell can be calculated, along with the work done by the cell on the next cell. If the work done by the cell exceeds the work done on the cell, then the cell has demonstrated power gain. In our experiment an input with one-half the normal potential swing was applied to the input. The resulting experiment demonstrated a power gain of 2.07, in agreement with theory [47].

Shift Registers

Clocking in QCA enables not only power gain, but also the control of the flow of information in the computational system, needed for data pipelining. The basic element in a data flow structure is the shift register. A QCA shift register consists of a row of cells controlled by different clock phases. In our experiment we fabricated a shift register of two cells. Although this is a very short shift register, it can be used as a long register. For our experiment we fabricated the two clocked QCA cells with electrometers coupled to each cell so that we could measure the polarization of each cell independently. In the experiment a bit of information is latched into the first cell, and the input removed. The bit is then copied into the second cell, and erased in the first. Then the bit is copied back into the first cell and erased in the second. In this way the bit is shifted between cells, just as it would be in a long shift register. The experiment demonstrated 5 bit transfers, limited only by thermally induced errors [48–50].

Fan-Out

An important element in a general logic system is fan-out, where the output of one element is sent to the inputs of two or more elements. Since the energy of the output is split, power gain in the following logic elements is needed to restore the signal level. To demonstrate fan-out in QCA we fabricated a circuit with three cells. In the

experiment the input is latched into the central cell, which then acts as an input to the top and bottom cells. When a clock is applied to the top and bottom cells the bit is copied into both cells, and full signal strength is produced in these cells [51], confirming the operation of the circuit.

3.3 Molecular QCA

Molecules represent the smallest artificial structures that can be engineered by humans. To form switchable QCA molecules, at least two charge centers are required that can be reversibly occupied or unoccupied by an electron. The field of mixed-valence chemistry [52] concerns itself with molecules that have at least two charge centers connected by a bridging group through which tunneling can occur. Ongoing investigation concerns the questions of what makes a good dot and what makes a good bridge.

Several early theoretical investigations used model electronic π-systems as dots [53–61]. These molecules are often radical ions containing unpaired electrons and would be very reactive and likely unstable in real systems. Their use was to establish the fundamentals. Electrons in molecules can exhibit bistable switching and the perturbation due to a similar molecule at a reasonable distance (such that the dots form a square) is sufficient to switch the molecule. Energy levels are such that these effects survive room temperature operation. Kink energies are large enough that molecular QCA is robust against variations in position and orientation of molecules. Groups surrounding the charge centers can effectively insulate them from conducting substrates but do not screen the field. Applied electric fields which vary at a much larger length scale can effectively clock molecules (with three appropriately arranged charge centers).

Molecular synthesis by the Fehlner [62–66] and Lapinte [67–69] groups have succeeded in creating molecules that show the requisite bistability. These dots use Fe and/or Ru charge centers. Electronic measurements of the Fehlner molecules attached to a surface showed distinctive bistable behavior as the electron was switched by an applied electric field. This demonstrated both the bistable character of the molecules, and the potential for clocked control of the charge configuration by an applied (and inhomogeneous) field. The Lapinte molecules have been imaged with STM by the Kandel group [67–70] and show the desired charge localization on one end of a symmetric double-dot molecule. Triple-dot molecules, of the sort required for clocked control, have also been made and imaged. More recently ferrocene-base double dot molecules have been made by the Henderson group and imaged by the Kandel group.

There is much chemistry yet to be understood in designing QCA molecules. One issue is what makes the ideal dot. Transition metal atoms have the advantage of using d-orbitals that participate less in bonding and so may be more isolated. Carbon-base π-systems, on the other hand, can be chosen such that they involve anti-bonding orbitals and may spread the charge out more and therefore yield a lower reorganization energy. The reorganization energy is the energy associated with the relaxation of the surrounding atoms and may in some cases trap the charge and inhibit switching. Creating appropriate bridging groups involves choosing a system that is either long enough or opaque enough to be an effective barrier to through-bond tunneling. Conjugated systems may be too conducting.

Another approach that combines single-atom realization with lithographic control is the STM-base lithography of the Wolkow group [71]. They have created room-temperature QCA cells using a remarkable approach involving removing single electrons from dangling bonds on a silicon surface. As with molecules, the single-atom sizes easily yield room temperature operation, yet the placement and orientation of the cells can be controlled lithographically using the STM tip.

3.4 Other Implementations

Nanomagnetic QCA was first introduced by Cowburn's group [72] and developed extensively by the Porod group [73] and the Bokar group [74]. The mapping from QCA cells that represent an electric quadrupole to those that represent a magnetic quadrupole is straightforward. Nanomagnetic implementations are discussed elsewhere in this volume.

Some have proposed cell-cell coupling based on an electron exchange interaction [75], and indeed the earliest calculations showed a small splitting between the singlet and triplet spin states [76]. This approach has two serious drawbacks: the exchange splitting is quite small, and it is zero if there is not tunneling from cell to cell. If there is tunneling from cell to cell, the information is no longer localized and spin-wave solutions predominate.

It is interesting to consider the fundamental question of what sort of systems could implement QCA action. There are two basic features of QCA that must be satisfied:

1. A bit is to be represented completely by the local state of a cell composed of atoms.
2. The interaction between cells is through a field, rather than by transport.

The cell's binary information must therefore be represented by the positional or spin degrees of freedom of the electrons and nuclei in the cell. Nuclear positions could be used to encode the information—for molecules this would entail a conformational change, for larger cells we would call it mechanical. Lighter mass electrons have an advantage in that they can switch positions faster than nuclei. Spin states of either nuclei or electrons could switch quickly.

The field connecting cells must be electromagnetic because the other candidate fields are either too short range (the nuclear strong or weak forces) or too weak (the gravitation force). Direct spin-spin interaction energies are very small, so for magnetic coupling we need many nuclear or electronic spins acting collectively. Nanomagetic QCA thus must be sufficiently large that the coupling is adequate at room temperatures. The direct Coulomb interaction is quite strong and allows molecule-to-molecule coupling between multipole moments of the charge distribution. Since by assumption there is no transport from cell to cell, the charge of the cell cannot change and higher moments must be used to encode the information. QCA thus far has used dipole coupling and quadrupole coupling—the difference being what one chooses to define as a cell. It is also possible to use contact potentials along the cell surface to coupled mechanical (nuclear) degrees of freedom. The possibilities then can be seen to reduce to these categories:

1. Mechanical cells coupled by electrostatic contact potential forces. These would suffer from the slower response of atoms compared with electrons, but remain largely unexplored.
2. Magnetic cells (collective nuclear or electronic spins) coupled by magnetic fields. This is the basis of nanomagnetic QCA described elsewhere in this volume.
3. Electronic cells coupled by Coulomb multipole-multipole interactions. The charge distribution could be the result of either mobile atoms or mobile electrons, and could involve a few or several charges.

Few-electron QCA cells, as has been noted above, have an intrinsic bistability due to charge quantization. If there are many charges forming the charge multipole, the bistability must be provided by another mechanism. One example is a CMOS cell that is an analog to QCA and switches adiabatically [77].

4 Issues in QCA Development

4.1 The Role of Quantum Mechanics in QCA

To achieve robustness against fabrication variations, the QCA paradigm uses only a classical degree of freedom, the electric (or magnetic) quadrupole moment of the cell. It does not use quantum phase information nor interference effects. QCA involves bits not qubits. It is quantum mechanical precisely in that it relies on quantum tunneling for cell switching. This is crucial because if quantum mechanics were "turned off" ($\hbar = 0$) there would be no tunneling and a QCA cell could not switch. If the barriers to tunneling were removed so that classical switching were allowed, a QCA cell would oscillate and settle into a particular configuration randomly depending on the details of the trajectory and energy dissipation. Switching a classical double-well system is much more prone to error because the system can get caught in a metastable state if the timing is not perfect. Reliance on quantum tunneling stabilizes the bit information.

4.2 Power Gain

In molecular, metal dot (discussed above), or other implementations, power gain is crucial because there is always some dissipation of energy as information moves from stage to stage in a computation. This dissipation is the microscopic version of friction in mechanical devices. It can be minimized, and by moving gradually can be reduced to whatever level is desired, but cannot be completely eliminated. Therefore, unless there is a way to restore the signal energy, it will eventually be completely attenuated. In conventional devices the source of the energy is usually the constant-voltage power supply. In QCA the restoring energy is provided by the clock; it automatically supplies enough energy to restore the signal levels.

4.3 Metastability, Memory, and Coherence

For a physical system to act as a memory its state cannot be determined by only its boundary conditions. A Hamiltonian system in a unique ground state, for example,

cannot act as a memory. A device with even short-term memory must therefore be in a metastable state. It could be in a state representing a 1 or be in a state representing a 0. Which state the device is in is depends not just on its boundary conditions, but also on its past. If there is a large enough kinetic barrier between these two states they can often be justifiably treated as distinct energetically degenerate states, but they are actually metastable states very weakly coupled and with a very long Rabi oscillation period.

In clocked QCA wires (i.e., shift registers), information is represented by bit packets, a few cells in the line that are polarized in the 1 or 0 state [78]. Since they could also be in the opposite state energetically, it is true that if the time evolution was completely unitary, the bit could quantum mechanically oscillate from one state to the other. There is a considerable kinetic barrier to doing that, however, just as in the case of a CMOS bit. Moreover, in real systems entanglement with the environment stabilizes the bit packet by loss of quantum phase in the system [79]. Decoherence is precisely this sort of entanglement with the environment and, though it is detrimental for quantum computing, it actually stabilizes QCA bits. Further exploration of the roles of environmentally-induced decoherence and energy dissipation are part of the broader question of the transition between the quantum and classical worlds.

4.4 Wire Crossings

QCA is naturally an in-plane technology; it does not require going out of the plane. How can one therefore cross wires, that is move one bit independently across the path of another? Several proposals have been made that accomplish this. (1) The original wire-crossing proposal was to use the symmetry of cells and the second-near-neighbor coupling (suitably strengthened by duplication) to allow one cell line to communicate across the path of another. The limitation here is the amount of control in placement and orientation required. (2) A permuter is a logical function which simply switches inputs A and B to output B and A. This can be done with logic, though it does take several cells to implement [80]. (3) With expanded clocking timing one can have one bit packet cross a wire intersection horizontally at one time, and vertically at a later time. The cost is in the added complexity of the clocking circuitry. (4) A bridge crossover, similar to the CMOS via structure can be constructed that takes QCA cells out of the plane to cross. (5) In many instances the crossing is for distribution of signals to different parts of a logic array. Tougaw and Khatun have designed a general matrix distribution scheme, again using augmented clocking patterns [81].

4.5 Computational Architecture

It is clear that QCA requires rethinking circuit and computer architecture on the basis of this new device paradigm. Nevertheless because QCA still supports Boolean logic function, it is natural that the first designs are taken over from usual logic circuitry. Much design work is underway, supported crucially by the design tool QCADesigner produced by the Walus group [82]. The goals of this important effort engaging many research groups are both to capitalize on the functional density that QCA cells allow

(molecular cells are ~1 nm square), and to exploit the clocking paradigm wherein all communication is via shift registers. Kogge and Niemier have been early pioneers of this [83–88], suggesting a universal clocking floorplan which supports general data-flow. Tougaw et al. [89] and Niemier et al. [90] have explored programmable QCA logic arrays, a promising area. Exploring QCA architectures and circuit ideas is a very active area, as witnessed by other contributions to this volume.

4.6 Lithograph and Self-assembly

QCA circuits need to have a designed layout that reflects the circuit function; entirely regular arrays do not have interesting behavior. As a consequence the information contained in the circuit layout must be imposed and this is usually done, as with all extant semiconductor circuits, through lithography. It is possible, however, to have self-assembly take care of constructing the dots and forming the dots into cells, and perhaps even forming the cells into lines or other functional groups. For molecular QCA, this is particularly promising because bottom-up self-assembly of molecules into supra-molecular structures is a common, albeit demanding, strategy. Building in some level of self-assembly from below, where the cell size is about 1 nm, and imposing circuit structure from above using lithographic techniques, which can reach below 10 nm, is an appealing match of technologies.

Another approach that has received some attention is to use DNA or PNA [91] self-assembled structures as "molecular circuit-boards." DNA structures with surprising amount of inhomogeneous patterning have been synthesized using Seeman tiles [92], or the more recent DNA origami techniques [93]. The long-range concept would be to engineering attachment sites in the DNA scaffold which would covalently bond appropriate QCA molecules or supramolecular assemblies [94–97]. The geometric information that defines the circuit layout would in this way be expressed through the sequencing of base-pairs that self-assemble into the scaffold. Many issues remain, of course, including the requirements of geometric matching to the DNA repeat distance and the polyanionic nature of DNA, which could interfere with QCA operation. PNA scaffolds are neutral and could potentially solve this problem.

4.7 Energy Dissipation

QCA has two fundamental motivators: ultra-small devices in large functional-density arrays, and low power dissipation. Power dissipation has been a major driver in every stage of the evolution of microelectronics. Adiabatic switching between instantaneous ground states allows the absolute minimum dissipation of energy to the environment. As Landauer [22] and Bennett [98] showed, there is no fundamental lower limit to the amount of energy that needs to be dissipated as heat in order to compute a bit of information. If information is erased, however, a minimum about of energy equal to $k_BT \log(2)$ must be dissipated. The combination of these two ideas is known as Landauer's Principle (LP) and is connected to the Maxwell Demon [99, 100]. Though there is a substantial consensus on the correctness of LP, it has come under criticism

from both industrial researchers [101, 102] and philosophers of science [103, 104]. The low power dissipation in QCA is an example of LP in action [105]. We have recently demonstrated experimentally that a binary switch can be operated with dissipation of 0.01 k_BT, in agreement with LP [106–108].

5 Future Prospects

QCA research activity continues on several fronts. Molecular QCA will require improved understanding of the chemistry of mixed-valence molecules. This includes exploring linker and dot moieties, the role of ligand relaxation in charge transfer, surface attachment and molecular-scale patterning. Significant progress in nanomagnetic implementations is reported by several other contributors in this collection. Metal-dot QCA deserves more exploration, even though it requires cryogenic operation. New fabrication methods may raise the operating temperature considerably. Exploration of circuits and computational architectures is crucial for fully exploiting the potential of locally interconnected nanodevices.

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