Quantum Cellular Automata: The Physics of Computing with Arrays of Quantum Dot Molecules

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Abstract

We discuss the fundamental limits of computing using a new paradigm for quantum computation, cellular automata composed of arrays of Coulombically coupled quantum dot molecules, which we term quantum cellular automata (QCA). Any logical or arithmetic operation can be performed in this scheme. QCA's provide a valuable concrete example of quantum computation in which a number of fundamental issues come to light. We examine the physics of the computing process in this paradigm. We show to what extent thermodynamic considerations impose limits on the ultimate size of individual QCA arrays. Adiabatic operation of the QCA is examined and the implications for dissipationless computing are explored.

1. Introduction

The ability to fabricate so-called zero-dimensional structures in which a few electrons can be artificially confined offers new possibilities for conceiving quantum computation at the nanometer scale. Such quantum dots have been fabricated with a variety of techniques: lateral surface gates producing fringing fields which further confine carriers in a two-dimensional electron gas, self-assembled semiconductor dots, chemically synthesized organic molecular structures, and many others [1]. In many cases, the occupancy of the "quantum dot atoms" can be well controlled so that quantum dot hydrogen, helium, lithium, and so forth can be created [2]. Recent experiments have shown that quantum dot atoms can be placed in close enough proximity to form quantum dot molecules [3].

We have considered whether, in the long run, a technology based on interacting quantum dot molecules might be feasible [4-8]. Considering not just individual devices, but an appropriate circuit architecture for

interconnecting such ultra-small structures has led us to focus on locally interconnected systems and in, particular, on cellular automata. Since at this size scale, coding information with currents or classical voltages is very problematic, we are led to a scheme in which the quantum dot molecular states themselves contain the information. A robust design is possible in which the Coulomb interaction between the molecular cells provides the intercellular interaction. Quantum coherence is only necessary across one cell.

In Section 2 we briefly review the quantum cellular automata (QCA) approach and emphasize its robustness. The approach does not require exquisitely tuned or finely balanced parameters. The physics of the intercellular interaction provides a non-linear response that plays the role of gain, resetting logic levels after each stage. In section 3 we mention the varieties of logic circuits that can be implemented using these ideas. Section 4 discusses in more depth the physics of how the computation is accomplished. In Section 5 we examine the role of entropy and how thermodynamic considerations limit the size of possible QCA arrays. In Section 6 we examine adiabatic QCA computation and attempt to use this concrete example of a quantum computer to illuminate the issues surrounding dissipation and reversibility.



Figure 1. A schematic of the quantum dot molecule which forms the basic cell for the QCA scheme. Tunneling is possible between any neighboring quantum dots. Simpler, four-dot cells are also possible.

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top gate

Figure 2. Cell occupancy stabilization. Because the various charge-states of the cell are well separated energetically, it is possible to stabilize the occupancy by using top and back gates to position the Fermi level so that all cells contain two electrons.

2. Quantum dot molecular cells

We consider the quantum dot molecular cell shown schematically in Figure 1 as the basic building block for the QCA architecture. Five quantum dots are close enough to enable electrons to tunnel between the dots. The barriers between cells are assumed sufficient to completely suppress intercellular tunneling. Each cell is occupied by two electrons. The occupancy can be stabilized because of the large energy splitting between different charge states of the cell. In most implementations, the cell occupancy is controlled by a top metal gate which covers all the cells and biases the cell such that the Fermi energy is between the doubly and triply occupied cell charge-states [2], as shown in Figure 2.

The Coulomb interaction between electrons in a cell acts to produce two distinct cell states with different charge configurations. If the barriers to tunneling are sufficiently high the two-electron ground-state wavefunction in the cell will localize the two electrons on antipodal sites. This localization is due to Coulomb exclusion [9], a phenomenon closely related to the wellknown Coulomb blockade of current, and results in nearly exact quantization of charge in each dot. There are two possible configuration with the electrons on opposite corners of the dot as shown in Figure 3. We define the



Figure 3. The two bistable states of the QCA molecular cell. Interaction between the electrons causes them to always be close to one of these two states.



Figure 4. The cell-cell response function. The polarization of the right cell is fixed and the induced polarization in the left cell is calculated by solving the twoelectron Schrödinger equation. The nonlinear nature of this response curve plays the role of gain in restoring signal levels from stage to stage. (After Ref. 7)

polarization of these two states to be +1 and -1 as shown in the figure. "Polarization" here simply indicates the alignment of charge along one of the cell symmetry axes, and does not refer to the appearance of a dipole moment. A polarization can be defined for a cell in an arbitrary (not necessarily completely polarized) state from the expectation values of the charge on each dot [4-8]. Here we will assume that the inter-dot tunnel barriers are sufficiently high that the we need only consider the completely polarized P = +1 or P = -1 states. In the absence of any potential from the environment the two polarization states of the cell are energetically degenerate. The presence of other charges in neighboring cells breaks the degeneracy and one polarization state becomes the cell ground state. Binary information can be encoded using the cell polarization. A cell polarization of +1 corresponds to a bit value of 1; a cell polarization of -1 corresponds to a bit value of 0.

The Coulomb interaction between cells causes the state of one cell to affect the state of a neighboring cell. Figure 4 show the polarization induced in one cell due to the presence of an adjoining cell. This cell-cell response curve is computed by solving the two particle Schrödinger equation for the cell in the presence of the potential asymmetry caused by the adjacent cell. The Hamiltonian is discussed in detail elsewhere [7]; we need mention here only that it includes the Coulomb interaction between electrons, the confining energy cost, and the tunneling between dots. The non-linear saturation of the cell-cell response function allows the physics to play the role that gain plays in conventional digital electronics. Even a slight polarization in a neighboring cell induces essentially complete polarization in the target cell. This means that at every stage (here every cell) the signal level is restored.





Figure 5. The robustness of the QCA binary wire. a) A line of cells is driven by the fixed polarization of the first cell. The nonlinear response is sufficient to completely polarize the line. It thus acts as a binary wire, transmitting information from one end to the other. b) The physical parameters of the cells are varied randomly down the wire. The inter-dot distance is *a* and the tunneling energy is *t*. Two of the cells have an extra electron in them. The nonlinear response between cells is sufficient to assure that the wire nevertheless functions properly. Note that the figures are not simply schematic, the dot size is proportional to the charge on the dot as calculated from a solution of the many-electron Schrödinger equation.

Figure 5 illustrates how this non-linearity enables a line of QCA cells to act as a robust binary wire. The first cell in the array is assumed to be kept in a fixed polarization state (for example by metallic electrodes that electrostatically lock in the cell state). The state of the other cells in the array is determined by self-consistent solution of the Schrödinger equation for the line. In Figure 5(a) the cells are all identical. The polarized state of the driver (first) cell induces the same polarization in all the cells in the line. In this way, the bit information is transmitted down the line which acts as a binary wire. In Figure 5(b), we have varied the barrier heights, cell sizes and occupancy (between 2



Figure 6. The QCA majority logic gate. Signals A, B, and C arrive through QCA wires and are fixed as the result of previous calculation. The device cell state is determined by the state of the majority of the three inputs. The output proceeds out to the right down a QCA wire.

electrons and 3 electrons) of the cells. The non-linear response between cells means that any degradation of the signal encoded in the cell polarization is quickly restored. The physics of the cell-cell interaction thus acts to make the transmission of information "forgiving" of imperfections in processing and irregularities in cell geometry; the QCA scheme does not require exquisite precision in balancing tunneling rates or other physical parameters.

3. Logical devices

The fundamental logical element in the QCA scheme is a 3-input majority logic gate. The gate, shown in Figure 6, is formed by the intersection of three wires whose logical states have been determined by the input. The output of the gate is not fixed. The state of the cell at the junction, which is the majority gate itself, will be identical to whichever logical state the majority of the three input lines are in. The output line simply transmits this state further. The threeinput majority gate can be reduced to a two-input AND or OR gate by setting one of its inputs to 0 or 1. We have shown elsewhere that wire bends, inverters, XOR gates, and planar wire crossings can be constructed. In each case the Schrödinger equation has been solved for the entire many-electron system self-consistently to verify that the design actually works. Any logical or arithmetic function can be implemented using this scheme. A single-bit full adder is shown in Figure 7 and serves as a specific example of how relatively complex, high functional units could be constructed.



Figure 7. A single bit full adder implemented in the QCA paradigm. The output S is the sum of bits A and B. The carry bit is C_i and the previous carry bit is C_{i-1} . Note that the figures are not simply schematic, the dot size is proportional to the charge on the dot as calculated from a solution of the many-electron Schrödinger equation. (After Ref. 7)

4. Computing in the QCA paradigm

Computing in the QCA paradigm is accomplished by the one-to-one correspondence between the unique manyelectron ground state and problem solution. The computing process is shown schematically in Figure 8. Input appears encoded in the cells along one edge of the QCA array; the output appears encoded in the cells at another edge. Initially, the system has the old values of input, in the figure labelled IN, at the input edge and the output corresponding to the solution of the previous problem, labelled OUT, at the output edge. The new computation begins by setting the input cells to their new values, labelled IN. Setting the state of these cells is presumably done electrostatically, and their state must be held to the IN values throughout the computation. Changing the state of the input cells requires work to be done on the array so immediately after, the array is in an excited state. The temporal evolution of the array from this point is quite complicated. Quantum oscillations and reflections occur, energy is dissipated to the environment through emission of phonons in the substrate, emission of plasmons in surrounding metallic gates, or other mechanisms depending on the specific details of the physical implementation of the dot structure. Modeling this transient phase of the calculation is extremely difficult and by design we choose not to use the details of this temporal evolution to accomplish the calculation. When this transient is over, in a characteristic relaxation time τ_{m} the system has dissipated the extra input energy and settles into its new ground state, appropriate to the new "boundary conditions" supplied by the input cells in state IN. When the system reaches this state, the output cells are in the new state OUT which properly encodes the solution to the computational problem. The state of the output cells can then be read non-invasively to reveal the computed solution.

In brief then, computation proceeds in three steps:

- i) Write the input bit by fixing the polarization state of cells along the input edge.
- ii) Allow the array to relax to its ground state while the new inputs are kept fixed.
- iii) Non-invasively read the results of the computation by sensing the polarization state of cells at the output edge.

This process requires two types of interaction between the macroscopic semiclassical world and the cells at the edge of the array. First, a *set* or *write* mechanism must be able to force the input cells into a specific polarization state. As mentioned above, this requires only electrostatic interaction with near-by conductors. Secondly, a *sense* or *read* mechanism must be able to detect the polarization of cells at the output edge without altering that polarization. That this is quite possible has been demonstrated experimentally in both metallic [10] and semiconductor quantum dot systems [11].

The QCA paradigm is *edge-driven* — both energy and information flow in from the edges of the array only. No contacts to interior cells are made directly. This eliminates the well-known interconnection problem. Furthermore, because there are no power rails, interior cells cannot be maintained far away from their ground state. The paradigm thus also involves *computing with the ground state*. Computation is accomplished by the mapping of the many-body ground state to the state representing the problem solution.

Conventional digital electronics features a high degree of input-output isolation which guarantees that information flows in one direction through a circuit and not in the reverse direction. What distinguishes input from output in the QCA paradigm? Examining the computational scheme described above for the specific



Figure 8. Schematic representation of computing cycle in QCA paradigm.

example of the full adder shown in Figure 7 illuminates the answer. The input side is determined by the fact that the input cells are held in a fixed polarization while the output cells are allowed to switch to whatever polarization lowers the overall system energy. In the transient phase of the calculation, information sloshes backward and forward through the whole array.

The full adder also illustrates an important point about the uniqueness of the many-electron ground state. Suppose the roles of input and output were reversed in the adder, that is, the cells corresponding to the sum and carry bit on the right in the figure were kept fixed and the cells at the left edge were unconstrained. Clearly, since several inputs could yield the same sum and carry, the resulting ground state is not unique. The uniqueness of the many-electron ground state is not a general property of an array of cells. It is a property of a QCA circuit that has been deliberately designed to yield a unique answer. The layout of the full adder illustrates the important fact that such a design is straightforward given the logical primitives available. The local nature of the cell-cell interaction means that hierarchical design rules are possible and one can understand the operation of a complex QCA design by analyzing the local components and how they are connected. Components can be pieced together --- one need not worry about solving the entire system as whole (although to verify this, we have in fact solved the entire many-electron problem).

The adder affords an example of the roles of physical and logical reversibility in this paradigm. As discussed above the QCA scheme uses dissipation to relax the excited system to the new ground state. It is thus fundamentally physically irreversible. This physical irreversibility permits the construction of logically irreversible circuits like the adder which have fewer outputs than inputs and so lose information in going from input to output. This contrasts with billiard-ball computers for which the physically reversible nature of the dynamics requires that only logically reversible circuits can be constructed. Running a billiard ball computer backward is equivalent to reversing the direction of a movie of the computation and allows unique recovery of the input states from the output states.

The QCA paradigm lacks time-reversal symmetry for a second more subtle reason which has nothing to do with energy dissipation. Suppose one knew the outputs of a particular QCA calculation and wanted to determine what the inputs were which produced them. One would hold the output cells in the desired polarization states and wait to see into which state the input cells settled. Physically, this does not correspond to time-reversing the original calculation since one has also changed the boundary conditions at the array edges. In the billiard ball computer input and output are distinguished only by the direction of time. In the QCA scheme input and output are distinguished by having different spatial boundary conditions. Running the calculation "backward" to determine inputs from outputs, thus does not correspond to playing a movie of the original calculation backward.

5. Thermodynamic considerations

The QCA paradigm relies on the physical array relaxing to its ground state to accomplish the computing. At nonzero temperatures, thermal fluctuations into excited



Figure 9. The cell response function for a cell driven on both sides at various temperatures. a) The response of the standard cell with inter-dot distance 20nm and relative dielectric constant 10. b) The response of a macro-molecular cell with inter-dot distance 2nm and relative dielectric constant 1.

states of the system may degrade the output into a thermal average of correct and incorrect results. Because there are no power rails to keep interior cells away from their thermodynamic equilibrium state, thermal effects will always be fatal to the scheme at high enough temperatures. In this section we examine these thermal effects, first for a single QCA cell, then for a linear array of cells.

5.1 Thermodynamics of a single QCA cell

We consider first a "standard" QCA cell with the dimensions and parameters discussed in detail in Ref. 7. The centers of the quantum dots in the cell are 20nm apart and the materials parameters are those of GaAs with a relative dielectric constant of 10. We compute a slightly different cell response curve than that in Figure 4 — the cell polarization P_1 induced when the cell is driven by *two* neighboring cells with polarization P_2 . This response function $P_1(P_2)$ is useful because it can be shown that a line of cells will polarize with a value of the polarization

given by the fixed point of repeated iterations of this response curve. We calculate this response curve at nonzero temperatures by calculating the thermal expectation value of the charge on each cell, averaging over all the excited states of the cell. The result is shown in Figure 9(a) for several values of the temperature. For temperatures up to about 7K, the curve is sufficiently nonlinear to enable interesting device performance. If we consider shrinking the cell size down to a macro-molecular level, possible operating temperatures increase. Consider the standard cell shrunk so that the inter-dot distance is 2 nm. Additionally, the relative dielectric constant we will now take to be unity since at the molecular level we no longer have screening by the semiconductor The corresponding results for the doubly-driven response function are shown in Figure 9(b). Acceptable nonlinearity now persists up to temperatures of about 700K.

5.2 Thermodynamics of a QCA array

For a line of cells and for a cellular array, the thermodynamic analysis must include consideration of both the spectrum of excited states of the array and the corresponding entropy.

Consider a line of N QCA cells, the binary wire, driven from one end by a cell fixed to a polarization of +1. The ground state consists of all cells with +1 polarization and it is non-degenerate. The ground state and the first two excited states are shown in Figure 10. In the first excited state, several cells line up properly with the driver but then a "kink" occurs and the subsequent cells all have the opposite polarization. The kink is energetically costly because neighboring cells have opposite polarization. The energy of a kink is, to a good approximation, independent of kink position and denoted Ekink. The kink can be in any position along the line resulting in a degeneracy of the first excited state of N-1 \approx N. The second excited state is a twokink state with energy 2 Ekink and has a degeneracy of roughly N². Generalizing to higher excited states is straightforward [12].

For a a non-linear array of cells, like the full adder, the situation is slightly different: the degeneracy is not exactly N (but of the same order), there may be some places where kinks cost somewhat less energy, and some kinks do not result in incorrect output states. Nevertheless we will make only small errors if we apply the results of the line analysis to the more general case.

As the number of cells increases the ground state remains unique and the separation between ground state and first excited state remain E_{kink} . However, the increasing degeneracy of the excited state means it is more and more likely that the system at nonzero temperature

will be found in an excited state — yielding a mistake. This can be quantified by considering the Helmholtz free energy of the system F = E-TS. The entropy of the nth excited state is

$$S_n = k_B n \ln(N). \tag{1}$$

The difference in free energy between the zero-kink and n-kink state is then

$$\Delta F_n = n E_{kink} \left[1 - \frac{k_B T}{E_{kink}} \ln(N) \right]$$
(2)

When this value ceases to be positive, the state with mistakes in the output cells becomes the thermodynamic equilibrium state. As long as this value is positive, the correct results appear at the output [13].

The result shows that for sufficiently large arrays the entropy term dominates and the QCA paradigm fails to produce a thermodynamic ground state corresponding to the correct calculational result. This consideration limits the size of arrays, but the logarithmic dependence on system size means that fairly large systems are still possible. Equation (2) shows the important parameter is the ratio (k_BT/E_{kink}), which can be reduced by either lowering the temperature or shrinking the cell size so that E_{kink} increases. If this ratio is 1/10, then N can be as large as 22,000; if this ratio is only 1/4, then N must be smaller than about 50.

In any case, it is clearly unrealistic to expect functioning arrays with as many elements as there are transistors in a modern microprocessor. The promise of the QCA paradigm lies in large high-function arrays which are surrounded with classical interface layers. This not only moderates the thermodynamic limits of a single superlarge array, but enables a classical latch to hold and store information reliably between QCA stages. This integration concept is illustrated schematically in Figure 11.

E = 2 E _{kink}	} *	*	r °	×	×	¥	×	×	×
$\mathbf{E} = \mathbf{E}_{kink}$	X		×.	×	*	×	×	×	¥
$\mathbf{E} = 0$	×	*	×	¥.	×	×	×	×	×

Figure 10. Ground state and first two excited states of a line of cells. The left-most cell is assumed fixed.



Figure 11. Schematic of several QCA arrays with classical interface layers.

6. Can QCA's compute without dissipation?

The QCA paradigm for computing with cellular arrays of quantum dots discussed above and illustrated in Figure 8 is clearly a dissipative one. It is possible to consider an alternative procedure of computing with a QCA array in which dissipation can be minimized [14]. We do not consider this scheme, which we call *adiabatic QCA computation*, to necessarily be a practical alternative, but examine it as a useful concrete example of quantum computing.

In adiabatic computation with QCA arrays we suppose that the barriers between quantum dots in the same cell can be lowered electrostatically and very slowly. The barriers between cells will remain high and fixed throughout. Consider for concreteness, that the inter-dot barriers are formed by the fringing fields of top-gate electrodes which are defining the quantum dots in a semiconductor twodimensional electron gas as shown schematically in Figure 12. Suppose the metal gates which control the intracell dot coupling are all connected together and held at a voltage Vg. When Vg is large and negative, the electrons in the cells are well-localized and the QCA cells function as described in section 2. If Vg is zero, the barriers between the dots vanish and the two cell polarization states will be energetically degenerate. The charge density in each cell then smears out into a large roughly circular distribution. Each cell has become a single quantum dot; the QCA array will no longer function.

The adiabatic QCA computation cycle proceeds as follows:

- Slowly (adiabatically) lower the magnitude of Vg and thus the inter-dot barriers so that each cell is completely unpolarized.
- ii) Slowly change the input voltages on the electrodes

that set the input cells. This takes no work because the input cells have both cell polarizations states degenerate.

- iii) Slowly raise the magnitude of V_g so that the cells repolarize into the new ground state appropriate for the new input state.
- iv) Read the results of the computation by noninvasively sensing the polarization of the cells at the output edge.

In step (i) the array does work on the circuit which controls the voltage source Vg. The same amount of energy is redelivered to the array from that circuit in step (iii). The only dissipation occurs as the charge which flows on and off the gate electrodes passes through the circuit resistance R of the voltage control circuit as shown in Figure 12. This resistance can be made arbitrarily small, so at least on an energy scale large compared to k_BT, the process can dissipate arbitrarily small amounts of energy. We can thus term it a macroscopically dissipationless process, meaning that the dissipation can be made as small as desired, down to an energy scale at which k_BT becomes significant. (Note that the energy separation between the correct ground state and the excited state can be much larger than k_BT when the output is read in step (iv); there is no problem in the read operation being successful in a thermal environment.)

Is it possible to operate the QCA adiabatically all the way down to energy scales of order k_BT ? That is, is the adiabatic QCA *microscopically* dissipationless? Clearly, if



Figure 12. Schematic of adiabatic switching of QCA array. The metallic gates which confine electrons to the dots are biased with voltage V_g . Barriers between cells are assumed to remain high. The input *i* is set by setting the voltage V_i . If V_g is adiabatically lowered before the input switching occurs, the only dissipation is through resistor R, which can be arbitrarily small, at least until energies become of the order of k_BT .

we can assume that the gate voltage Vg can be slowly and smoothly lowered until the energy separation between the ground state and excited state of each cell is actually zero, then this is indeed microscopically dissipationless. But is this physically reasonable? The focus of the argument then becomes the process of smoothly charging and discharging the gate electrodes, which are capacitively coupled to their surroundings with capacitance C, through the circuit resistance R. When gates are discharged to the point where $CV_g^2 \approx k_B T$, can the process continue adiabatically? We suggest that perhaps it cannot. At that point thermal fluctuations in the current through resistor R will be sufficient to suddenly (non-adiabatically) change the voltage on the gates. The two-electron system in the cells must now dissipate kBT to the environment and not simply transfer energy reversibly to the circuit. We believe that this examination focuses attention where it is due: at the interaction between circuit system, and thermal environment when energy scales become comparable to thermal fluctuations. A further detailed analysis of this problem is needed.

This analysis, which shows that adiabatic QCA computation is macroscopically dissipationless is particularly interesting in light of the issue of logical reversibility. Notice, for example, that the full adder circuit could be operated in this adiabatic regime. Thus it provides an example of an implementation of a logical irreversible function in a macroscopically dissipationless system.

7. Conclusion

Quantum cellular automata present an interesting case of potentially useful quantum computing exploiting the emerging technology of quantum dot fabrication. The physics of inter-dot coupling provides bistability so that the scheme is robust and tolerant of fabrication variations. Because QCA computing uses the ground-state of the many-electron system to map onto the encoded problem solution, it has limits imposes by thermodynamics. In particular, for a given characteristic "mistake energy", we have called Ekink, there exists a maximum array size beyond which entropy will cause mistakes to be thermodynamically favorable. QCA arrays can be implemented in an adiabatic computation mode which is certainly macroscopically dissipationless. It is an open question as to whether the limit of zero dissipation can actually be achieved in a thermal environment.

Finally, we note that the QCA paradigm presented here contains no provision for memory storage. It therefore does not represent a universal computer, but rather a universal arithmetic or logical function evaluator.

Acknowledgments

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