

PhD Thesis

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## Chapter 1

# Introduction



## Chapter 2

# Quantum-dot cellular automata

Lent et al. introduced the concept of quantum-dot cellular automata as an alternative computing paradigm in 1993 [1]. Thus the aim was a novel physical scheme to build digital circuits that would overcome some of the limitations of CMOS technology, promising potentially lower power consumption, higher device density, and faster clocking. As the name alludes to, quantum-dot cellular automata (QCA) is built from quantum-dots which are grouped together in cells. Figure 2.1(a) shows a basic QCA cell. Four quantum dots are arranged on the corners of a square. The dots are idealized as perfectly localized single orbitals on a perfectly decoupled non-intrusive medium. Therefore, each dot can be occupied by up to two electrons. In the QCA scheme, however, each cell is occupied by only two electrons in total. The cell is quarter-filled. The electrons tunnel between different dots in a cell, but the dominant energy scale is set by the Coulomb repulsion between the particles. Simply by virtue of the Coulomb repulsion, and ignoring the comparatively small tunnelling for now, the diagonal states, Fig. 2.1(a), are the two energetically preferred electron configurations. In comparison, edge states or doubly occupied quantum dots are unfavourable higher energy states, Fig. 2.1(b). A priori the two diagonal states are energetically degenerate, but this degeneracy can be lifted by introducing an external Coulomb potential, for example a second nearby QCA cell. Then these two states can be identified with logic 0 and 1, as indicated in the figure.

A single cell by itself is, of course, not very interesting. Thus, multiple cells can be positioned next to each other, for example as a straight line of cells, Fig. 2.1(c). The approach now again assumes that Coulomb is the driving force and that electron tunnelling between cells is very small and ideally zero. For a straight line of cells, these long-ranging, unscreened Coulomb forces will tend to align the electron configurations of adjacent cells. If the first cell is in logic state 1 then the second cell will also prefer logic state 1 and so will in turn all the other cells in the line. The situation is the same for logic state 0. Therefore, a straight line of cells is similar to a wire not only in geometry, but also in functionality: It transmits a digital signal. The same is true, with slight modifications, for a diagonal

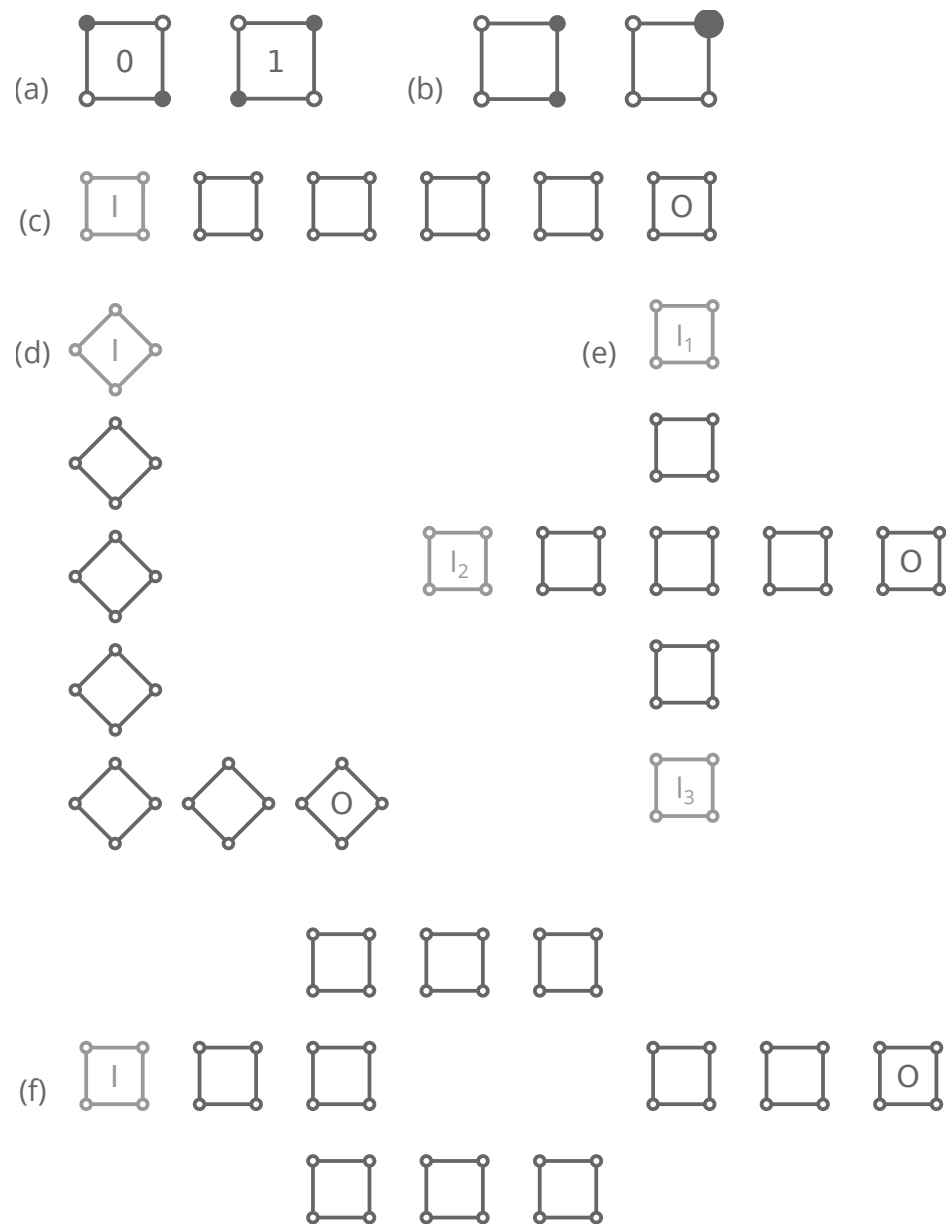


Figure 2.1: ...



line of cells — cells rotated by  $45^\circ$ —, Fig. 2.1(d). In this case the signal alternates from cell to cell, that is, logic 1 will follow logic 0 which followed from logic 0, and this again is simply by virtue of the dominant Coulomb interactions between electrons on different cells. By using an even number of cells the diagonal line of cells works as a wire just as well as a straight line of cells. The pictogram also demonstrates a  $90^\circ$  for the diagonal line of cells which our newly gained intuition for these Coulomb-driven systems expects to pose no problem for signal transmission.

The main idea of the QCA approach becomes apparent: Ideally bistable cells interact with each other solely by Coulomb repulsion. By arranging the cells in clever geometries we can realize interesting functionalities. The idea as such is quite general and does not strictly rely on the two-electron-four-dot cell introduced above. Indeed, a number of variations exist, such as one-electron-two-dot cells, interacting via dipole fields instead of quadrupole fields as for the conventional cells, or four-dot cells with six electrons—two holes—instead of two electrons. Even the interaction need not be Coulombic. For example, magnetic QCA schemes have been explored. While QCA carries “quantum” in its name and is sought to be implemented at the nanoscale, the approach operates close to the classical limit. The Coulomb interaction is absolutely dominating with the tunnelling of electrons a small perturbation, which nonetheless drives the system’s dynamics. The approach is insensitive and in fact ignores the spin degree of freedom. Let us finally note that QCA is not a cellular automata in a strict mathematical sense, but only by analogy to the idea of interacting cells.

One clever geometrical cell arrangement is the majority gate, Fig. 2.1(e). The gate has three inputs which “vote” on the central cell. The majority wins and sets the single output. The device is commonly operated with one fixed input, for example  $I_3 \doteq 0$  or  $I_3 \doteq 1$ . In the first case,  $I_3 \doteq 0$ , the device functions as an AND gate for the remaining two inputs,  $O = I_1 \wedge I_2$ . In the second case,  $I_3 \doteq 1$ , it is an OR gate with  $O = I_1 \vee I_2$ . Now, the only missing piece for Boolean algebra is negation,  $O = \neg I$ . We had already seen that simply arranging cells at an  $45^\circ$  angle as in the diagonal line of cells above negates the signal from cell to cell. The inverter, Fig. 2.1(f) recasts this idea into a more robust layout. With that we have, at least in principle, all the necessary building blocks for Boolean algebra and thus digital circuitry.

Conceptually, it is most elegant to set the inputs to a QCA circuit via driver cells — cells that resemble the QCA cell in form, but are made up from static point charges instead of quantum dots. These static charges are thought to be manipulatable to vary the input smoothly from the logic 0 to the logic 1 state. In figure 2.1 these driver cells are represented in light grey. Of course, in practice such driver cells would be difficult if not impossible to implement and the input would more likely be set by leads that provide the necessary perturbative electrostatic field. The output of a QCA device can be directly read from its output cells. In practical implementations this will require a non-trivial charge probing apparatus.

Changing the input for a QCA device throws the system into an excited, non-equilibrium

state. The system will then dissipatively propagate to its new ground state. For the given inputs, this ground state corresponds to the solution of the computational problem the circuit is designed to solve. Let us emphasize this: In QCA, the computational solution maps directly to the physical ground state! At all times during performing a computation, the system is relatively close to its ground state. Only a few charges move locally, in each cell. QCA is a truly current-free approach and consequently inherently low-power, especially when compared with CMOS technology. But the operation close to the ground state also raises concerns for the operational temperature for these devices. It is clear that for applications we would want to engineer the system so that the energy gap between the ground state and the low-lying excited states far exceeds room temperature.

It is difficult to derive general expectations for the clocking speed of QCA circuits. The switching speed of a majority gate, for example, will greatly depend on the system's parameters, but particularly on the nature of the dissipative coupling of the circuit to its environment. A small dissipative coupling will have the output polarization oscillating before it eventually settles to its correct value. A very dissipative system in contrast might get stuck in meta-stable states. Different material systems provide different dissipative channels and modelling them quantitatively or even qualitatively correctly is very challenging.

QCA circuits consist of wires, gates, and other structures arranged on a two-dimensional surface—very similar to conventional electronics devices. However, the structures themselves are quasi-one-dimensional and this poses a challenge for building large-scale QCA circuits. A good example is a single long wire, which is truly one-dimensional. Generally, a one-dimensional system cannot be ordered in the thermodynamic limit except at zero temperature. Therefore, the finite-temperature infinitely long wire will always have at least two different domains, logic 0 and logic 1 (assuming perfectly bistable cells for simplicity), and thus not be able to transmit a signal. When we think about switching the input for the wire, we think of the information being propagated as a charge density wave throughout the wire, or, equivalently, as propagating the domain boundary between logic 0 and logic 1. This domain boundary incurs an energy cost that the system seeks to minimize. For an increasingly longer wire, however, the gain in entropy for moving the domain boundary freely throughout the wire ( $S \sim \log N$ ,  $N$  the number of cells) soon exceeds the loss in energy, which is reflected by the free energy of the system,  $A = U - TS$ . Consequently, the gap between the first excited state and the ground state and the desired operational temperature will determine the maximum system size.

To address this scaling problem we partition large circuits into smaller units. Each unit can be turned “on” and “off” separately: Individual gates allow to control the electrostatic potential for each unit, effectively raising and lowering the tunnelling barriers between quantum dots and thus allowing to freeze or delocalize the electrons. A unit with *frozen* electrons can serve as the input for a unit with more *active* charge carriers, which works like a regular QCA circuit. A unit with completely *delocalized* electrons, in contrast, will not influence adjacent units. By putting each unit through the three phases *delocalized*, *active*,

and *frozen* and synchronizing adjacent units appropriately, we can control the information flow through the system very nicely, as illustrated in Fig. TODO. Therefore, by partitioning the circuit and introducing a clocking scheme we not only handle the scaling problem, but also arrive at a pipelining architecture that greatly improves the control over information flow in the system. Of course, in practice the QCA circuit units cannot be too small as they must be individually addressable. Gates which turn QCA units “on” and “off” also provide another potential benefit. We are able to control how and especially how fast the gate voltage is changed and should be able to tune it with respect to the inherent time-scales of the QCA system, which are set by the system’s parameters and the dissipative coupling to its environment. This should allow a better control over the dynamics of the switching process.

QCA systems are typically modelled by an extended Hubbard Hamiltonian. The Hubbard model originated in the early 1960s to describe rare-earth systems with highly localized d- and f-electrons and has since then, of course, become one of the most widely studied and successful models in condensed matter physics. In basing our description on the Hubbard model we already put some key assumptions in place. For example, we assume that the quantum dots are similar to the highly localized d-orbitals. Depending on the particular QCA implementation this might or might not be a good description. However, our interest is not in the precise details of any particular material system QCA might be implemented on, but our aim is to investigate universal characteristics of QCA systems. An idealized but semi-realistic description is what we want and for that the Hubbard model is indeed an appropriate—and tractable—starting point. Specifically, the Hamiltonian we use is

$$H = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma} + \sum_{i<j} V_{ij} (n_{i\uparrow} + n_{i\downarrow} - q) (n_{j\uparrow} + n_{j\downarrow} - q) , \quad (2.1)$$

where  $c_{i\sigma}^\dagger$  ( $c_{i\sigma}$ ) creates (annihilates) an electron on quantum-dot  $i$  with spin  $\sigma$  and the particle number operator is  $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ ;  $t_{ij}$  is the overlap integral between dots  $i$  and  $j$ ,  $U$  is the Hubbard on-site Coulomb repulsion,  $\mu$  the chemical potential, and  $V_{ij}$  the long-ranged Coulomb interaction, which is characteristic for QCA systems. For simplicity the Coulomb term is chosen to be  $V_{ij} = \frac{1}{r_{ij}}$  where  $r_{ij}$  is the distance between the two dots  $i$  and  $j$ . We also introduce the *compensation charge*  $q$  which is thought to represent a possible positive ion at each quantum dot site. This constant positive charge allows us to tune the net cell charge. For two electrons per cell, for example,  $q = 0$  yields a net cell charge of  $-2e$  whereas  $q = \frac{1}{2}$  represents zero net cell charge, and here the cell becomes a perfect electrostatic quadrupole.

The geometric layout of the QCA system and therefore its functionality is encoded in the hopping parameter  $t_{ij}$  and the long-ranged Coulomb term  $V_{ij}$ . For the hopping parameter we usually only consider nearest-neighbour hopping and specifically no hopping between the cells. While this constraint is not strictly necessary for QCA, it is in line with the approach’s underlying idea and greatly simplifies calculations. Because the overlap

integral decays exponentially with distance, as long as the distance between dots from different cells is larger than the distance between dots within one cell, the assumption will introduce only a small error. Still, this is something to keep in mind if we place cells very close to each other. Note that without inter-cell hopping we can decompose the Hamiltonian into purely Coulombic cell-cell interaction terms  $H_{kl}$  and single cell terms  $H_k$  which capture the kinetics as well as the inside-cell Coulomb interactions,

$$H = - \sum_k H_k + \sum_{k < l} H_{kl} , \quad (2.2)$$

where  $k$  and  $l$  number the cells.

To parameterize the Coulomb term  $V_{kl}$  and specifically  $r_{ij}$ , the distance between quantum-dots  $i$  and  $j$ , we introduce the cell edge length  $a$  and the cell-cell distance  $d$ , as illustrated in Fig. TODO where we have used a short line of cells as an example QCA system. The angle between adjacent cells is denoted by  $\theta$ . Ideally each cell should be in logic state 0 or logic state 1, but, of course, in practice a cell can be in any superposition of the two states or even in a different state altogether. The *cell polarization*  $P_k$  quantifies the state of the cell,

$$P_k = \frac{1}{2} (n_{4k+2} + n_{4k+4} - n_{4k-1} + n_{4k-3}) , \quad (2.3)$$

where the dots in each cell are numbered clockwise as indicated in the figure. The cell polarization is  $P_k = -1$  for a logic 0 and  $P_k = +1$  for a logic 1 state. Without any external input the polarization of a cell will be  $P_k = 0$ . In the example line of cells, the input is set via the driver cell's polarization  $P_D$  at the left end. The driver cell's four static point charges are adjusted to reflect the desired polarization  $P_D$ . For QCA, the cell polarization really is the observable of utmost interest. It indicates whether a cell is in logic state 0 or logic state 1 and how polarized the cell is, where ideally, of course, the cell should always be fully polarized  $|P_k| = 1$ . In short, the cell polarizations will indicate how well the QCA approach works for a given system and, unsurprisingly, calculating cell polarizations for various geometric layouts over a wide range of system parameters will be our main focus.

TODO: Somewhere I need to talk more about temperature, maybe. (more details: idealized; no substrate; no screening – maybe discuss this with the Silicon system) Emphasize somewhere that by using the Hubbard model our calculations and results might not be applicable to QCA implementations that are decidedly not well-described by Hubbard physics.

## Chapter 3

# Approximations



# Bibliography

- [1] C. S. Lent, P. D. Tougaw, W. Porod, and G. H. Bernstein, “Quantum cellular automata,” *Nanotechnology* **4** (1993) 49.