

Signal Processing with Near-Neighbor-Coupled Time-Varying Quantum-Dot Arrays

Árpád I. Csurgay, *Fellow, IEEE*, Wolfgang Porod, *Senior Member, IEEE*, and Craig S. Lent

Abstract—The Nano-Devices Group at the University of Notre Dame proposed a new device that encodes information in the geometrical charge distribution of artificial (or natural) molecules. Functional units are composed by electrostatic coupling. In these units, processing takes place by reshaping the electron density of the molecules, and not by switching currents [1]. Signal processing potential of next-neighbor-coupled cellular nonlinear networks (CNN's) has been recently explored with the conclusion that local-activity of the cells is necessary to exhibit complexity [2]. It will be shown that Coulomb-coupled time-invariant artificial molecules behave like nonlinear locally passive devices, thus signal-power-gain or multiple equilibria cannot be achieved by integrating them. However, the signal input-output relation of strongly nonlinear molecules can be varied in time by adiabatic pumping, called clock control. It will be shown that strongly nonlinear time-varying molecules can transform the necessary amount of clock energy into the signal flow, thereby enabling the network of molecules to perform signal processing.

I. INTRODUCTION

NANO-ELECTRONICS faces three major challenges:

- 1) the emergence of new and macroscopically visible quantum phenomena;
- 2) integration via equipotential wires deteriorates device performance, thus system integration needs new approaches;
- 3) as device size shrinks the increasing power dissipation becomes intolerable.

The physics and fabrication technologies of nanostructures are reasonably well understood. Chemists and both experimental and theoretical physicists have been recently and are continuously exploring the meso-scale. A large variety of discrete nanodevices have been proposed and built, but still a large gap exists between device physics and nanoelectronic systems integration. In order to create a viable integrated nanosystem, the three major challenges mentioned above must be coherently addressed.

The Nano-Devices group of the Electrical Engineering Department at the University of Notre Dame has been studying

the potential engineering applications of meso-scale physics for more than a decade. According to the Notre Dame proposal:

- 1) quantum phenomena (tunneling, discrete molecular spectra) should and could be used for nanoscale signal processing;
- 2) near-neighbor-coupled cellular networks are promising as architectures for nanoelectronic processors;
- 3) dissipation could be radically decreased by encoding information into the ground state geometrical charge distribution of artificial (or natural) molecules, and composing functional units by electrostatic coupling. In these units, processing takes place by reshaping the electron density of the molecules, and not by switching electron currents.

In order to design large-scale integrated nanosystems a hierarchy of models has to be established from device dynamics to system functions. In case of large-scale systems composed of strongly coupled quantum devices, the accurate modeling is a formidable task. In this paper, we restrict ourselves to a molecular array which can be described by a restricted class of models. We assume that the array is composed of quantum devices, called “molecules,” whose internal dynamics can be approximated by a finite-state model, but the molecules are far enough from each other; thus, a classical model of the intermolecular forces is accurate enough. This assumption results in a semiclassical approach.

However, the density matrix or equivalently the coherence vector description of the internal dynamics of this restricted class results in a set of coupled nonlinear differential equations. The state equations of a coupled molecular array show strong similarities to nonlinear circuit equations. An analogy between the voltage-current relationship of n -ports and the coherence vector-Hamiltonian relationship of two-state molecules will be recognized. This analogy helped us to identify locally passive and locally active molecular arrays, which give an important insight into the realizability of integrated nanosystems.

II. QUANTUM-DOT CELLULAR ARRAY: QCA

A scheme for computing with networks of coupled quantum dots has been proposed [1]. The physical mechanisms for interactions between the dots are the Coulomb interaction and quantum-mechanical tunneling.

To illustrate the proposal let us consider an artificial “molecule” encoding information in its geometrical charge configuration containing four quantum dots (electron sites) as schematically shown in Fig. 1. The dots are shown as the open circles which represent the confining electronic potential. Let us assume that the “molecule” is occupied by two electrons, which

Manuscript received November 24, 1998; revised March 6, 2000. This work was supported in part by a joint grant of NSF (National Science Foundation INT96-15 497) and HAS (Hungarian Academy of Sciences OTKA T-016 515), and also by the Office of Naval Research.

Á. I. Csurgay is with the Center for Nano Science and Technology, University of Notre Dame, Notre Dame, IN 46556 USA, on leave from Technical University of Budapest, Budapest, Hungary.

W. Porod and C. S. Lent are with the Center for Nano Science and Technology, University of Notre Dame, Notre Dame, IN 46556 USA.

Publisher Item Identifier S 1057-7122(00)06340-6.

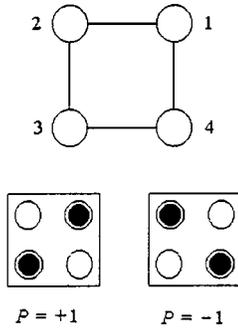


Fig. 1. Four quantum dot two-state artificial molecule.

are schematically shown as the solid dots. The electrons are allowed to “jump” between the individual quantum dots in a molecule by the mechanism of quantum mechanical tunneling. Tunneling is possible on the nanometer scale when the electronic wave-function sufficiently “leaks” out of the confining potential of each dot, and the rate of these jumps may be controlled during fabrication by the physical separation between neighboring dots or by a confining potential. The two electrons experience their mutual Coulombic repulsion, yet they are constrained to occupy the quantum dots. If left alone, they will seek, by hopping between the dots, the configuration corresponding to the physical ground state of the cell. It is clear that the two electrons will tend to occupy different dots because of the Coulomb energy cost associated with bringing them together in close proximity on the same dot. It is easy to see that the ground state of the system will be an equal superposition of the two basic configurations with electrons at opposite corners, as shown in the figure.

We may associate a “polarization” with a specific arrangement of the two electrons in each molecule. Let us label the four dots in the following fashion: starting from the upper right-hand corner, we label the dots in the four corners from 1 to 4. We also denote the electron density in dot j by ρ_j , with the constraint that in each cell, the sum of all the dot occupancies ρ_j has to add up to a total of two electrons. With that, we can define a molecule’s polarization as

$$P \equiv \frac{(\rho_1 + \rho_3) - (\rho_2 + \rho_4)}{\rho_1 + \rho_2 + \rho_3 + \rho_4}. \quad (1)$$

Note that this polarization is not a dipole moment, but a measure for the alignment of the charge along the two diagonals. A polarization of $P = +1$ results if cells 1 and 3 are occupied, while electrons on sites 2 and 4 yield $P = -1$. Any polarization between these two extreme values is possible, corresponding to configurations where the electrons are more evenly “smeared out” over all dots. The ground state of an isolated molecule is a superposition with equal weight of the two basic configurations, and therefore has a net polarization of zero.

This configuration has been studied by solving the Schrödinger equation using a quantum mechanical model Hamiltonian [5]. For the relevant literature see also [9] and [15]. A Hamiltonian of the extended Hubbard type was used to describe the QCA cell, or “molecule” as we call it. Each quantum dot was treated as an electron site. About the details, we refer to the literature, but suffice it to say that the equation

of motion depends on the quantized energy levels of each dot, the coupling between the dots by tunneling, the Coulombic charge cost for a doubly occupied dot, and on the Coulomb interaction between electrons in the same molecule, and also with those in neighboring molecules.

The solution of the Schrödinger equation, using molecule geometry with experimentally reasonable parameters, confirmed the intuitive understanding that the ground state is a superposition of the $P = +1$ and $P = -1$ states. In addition to the ground state the Hamiltonian model yields excited states and molecule dynamics.

Weakly coupled molecules have also been studied. The two polarization states of a molecule will not be energetically equivalent if the molecule is in a nonuniform electric field, if, e.g., other molecules are nearby. It has been assumed that the molecules are far enough apart that the overlap between their wavefunctions can be ignored, i.e., only intramolecular tunneling takes place, and there is no electron exchange between molecules [23]. With these assumptions the extended Hubbard-type model has been studied for two molecules, and also for one and two-dimensional (2-D) arrays of molecules.

Extensive studies have been performed to understand the dynamics of weakly coupled arrays composed of cells built on specific material systems. The studies have indicated that a two-state model describing the dynamics of individual molecules, together with an intermolecular force model at the level of the Hartree–Fock approximation are leading to promising models. These approximate models can be used to simulate integrated networks of weakly coupled two-state molecules.

III. THE TWO-STATE APPROXIMATION

We assume that the molecular array will perform ground-state signal processing. This proceeds in three steps:

- 1) first, the initial data is set by fixing the polarization of those cells at the edge, which represent the input information (“edge-driven” computation);
- 2) next, the whole array is allowed to relax (or it is adiabatically driven) to the new ground state, compatible with the input cells kept fixed (computing with the ground state);
- 3) finally, the results of the computation are read by sensing the polarization of those cells at the periphery which represent the output data.

Thus, we have assumed that the dynamics of our array is always close to the ground state, and we can rely on the two-state approximation. We describe the quantum state of a molecule using two basis states $|\varphi_1\rangle, |\varphi_2\rangle$ which are completely polarized

$$|\Psi\rangle = \alpha|\varphi_1\rangle + \beta|\varphi_2\rangle, \quad \Psi = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}. \quad (2)$$

Here α and β form a complete set of probability amplitudes. The probability of finding the molecule in state $|\varphi_1\rangle$ as an outcome of a measurement is $|\alpha|^2$, and finding it in state $|\varphi_2\rangle$ is $|\beta|^2$. Assuming that the two basis states are the only admissible eigenstates, we get

$$|\alpha|^2 + |\beta|^2 = 1. \quad (3)$$

Using α and β , the polarization defined above is given by

$$P = |\alpha|^2 - |\beta|^2. \quad (4)$$

If there are a set of molecules arranged on a two-dimensional (2-D) array, and tunneling is restricted to the interior of the molecules, then the Coulomb interaction between adjacent molecules increases the energy of the configuration if the polarizations differ. This can be accounted for by including an energy shift corresponding to the weighted sum of the neighboring polarization. We define this weighted sum for molecule k as follows

$$\bar{P}^{(k)} = \sum_{j \in S^{(k)}} w(\mathbf{R}^{(k)} - \mathbf{R}_j) P_j \quad (5)$$

where the sum is over an appropriate neighborhood $S^{(k)}$ around the molecule k . The weights can be calculated directly from the Coulomb interaction between the molecules. In the presence of other molecules, the energy of the two basis states becomes different. The Hamiltonian for each molecule can then be written as

$$H^{(k)} = \begin{bmatrix} -\frac{1}{2}\bar{P}^{(k)}E^{(k)} & -\gamma \\ -\gamma & \frac{1}{2}\bar{P}^{(k)}E^{(k)} \end{bmatrix} \quad (6)$$

where γ is the interdot tunneling energy and $E^{(k)}$ is the electrostatic energy cost of two adjacent fully polarized molecules having opposite polarization. If we assume that there are no quantum entanglements between molecules and no dissipative contact with the environment, then the dynamics of the array is simply given by a set of coupled Schrödinger equations for each molecule:

$$j\hbar \frac{\partial}{\partial t} |\Psi^{(k)}\rangle = \mathbf{H}^{(k)} |\Psi^{(k)}\rangle. \quad (7)$$

This approach treats the exchange and correlation effects exactly within each molecule and treats intermolecular interactions at the level of the Hartree–Fock approximation.

Without loss of generality, α can be considered real because the spinors

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad \text{and} \quad e^{j\delta} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

represent the same state for any real δ . Thus, the state is represented by two real variables, $-1 \leq \alpha \leq 1$, and the phase of β

$$\Psi = \begin{pmatrix} \alpha \\ \sqrt{1 - \alpha^2} e^{j\varphi} \end{pmatrix}.$$

However, we can express α and $|\beta|$ as a function of P

$$\alpha = \sqrt{\frac{1+P}{2}} \quad \text{and} \quad |\beta| = \sqrt{\frac{1-P}{2}} \quad (8)$$

thus the polarization P and the phase angle φ can be introduced as new state variables [6], and (7) can be transformed to

$$\hbar \frac{dP^{(k)}}{dt} = -2\gamma \sqrt{1 - P^{(k)2}} \sin \varphi^{(k)} \quad (9)$$

$$\hbar \frac{d\varphi^{(k)}}{dt} = -\bar{P}^{(k)} E^{(k)} + 2\gamma \frac{P}{\sqrt{1 - P^{(k)2}}} \cos \varphi^{(k)} \quad (10)$$

where $P^{(k)}$, $\varphi^{(k)}$ are the polarization and phase of the k th molecule, and $\bar{P}^{(k)}$ represents the effect of the neighboring molecules on the k th one according to (5). State equations (7) and (9) and (10) are inherently lossless and the phenomena of relaxation to ground-states are not taken into account.

IV. DENSITY MATRIX DESCRIPTION OF MOLECULAR ARRAYS

An alternative description of the state of a molecule is to characterize it by the density operator (or density matrix)

$$\rho = |\Psi\rangle\langle\Psi| = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} (\alpha^* \beta^*) = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix}. \quad (11)$$

Note that ρ is Hermitian and the sum of its diagonal elements is one

$$\text{trace}(\rho) = |\alpha|^2 + |\beta|^2 = 1. \quad (12)$$

Every 2×2 matrix can be expanded as

$$\rho = \lambda_0(\mathbf{1} + \lambda_x \sigma_x + \lambda_y \sigma_y + \lambda_z \sigma_z) \quad (13)$$

where $\mathbf{1}$ is the 2×2 unit matrix, and σ_x , σ_y , and σ_z are the Pauli matrices

$$\begin{aligned} \sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, & \sigma_y &= \begin{pmatrix} 0 & -j \\ j & 0 \end{pmatrix} \\ \sigma_z &= \begin{pmatrix} -1 & 0 \\ 0 & +1 \end{pmatrix}. \end{aligned} \quad (14)$$

If ρ is Hermitian $\lambda_0, \lambda_x, \lambda_y, \lambda_z$ are real numbers, and if $\text{trace}(\rho)$ is 1, then $\lambda_0 = 1/2$. From (11) and (13), we get

$$\begin{aligned} \lambda_x &= 2\text{Re}(\alpha^* \beta); & \lambda_y &= 2\text{Im}(\alpha^* \beta) \\ \lambda_z &= |\beta|^2 - |\alpha|^2. \end{aligned} \quad (15)$$

Let us introduce a three-dimensional (3-D) vector $\vec{\lambda}$ whose components are $\lambda_x, \lambda_y, \lambda_z$, respectively. Note that the polarization P introduced above is $-\lambda_z$, and $\lambda_x = \sqrt{1 - P^2} \cos \varphi$, $\lambda_y = \sqrt{1 - P^2} \sin \varphi$, thus

$$\vec{\lambda} = \begin{pmatrix} \sqrt{1 - P^2} \cos \varphi \\ \sqrt{1 - P^2} \sin \varphi \\ -P \end{pmatrix} \quad (16)$$

and

$$|\vec{\lambda}|^2 = \lambda_x^2 + \lambda_y^2 + \lambda_z^2 = 1. \quad (17)$$

Let us chose $\vec{\lambda}^{(k)}$, called coherence vector [7], as the state-variable of molecule k . Thus, the state is represented by a 3-D vector of unit length, and the dynamics of a lossless molecule is described by the time-varying direction of the $\vec{\lambda}$ vector. Note that the number of independent state variables is again two.

We have seen that the dynamics of the probability amplitudes is determined by the time-dependent Schrödinger equation (7)

$$j\hbar \frac{d}{dt} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \quad (18)$$

We also know that

$$j\hbar \frac{\partial}{\partial t} \rho = \mathbf{H}\rho - \rho\mathbf{H}.$$

Substituting (13) into this equation and solving it for the time derivatives of $\lambda_x, \lambda_y,$ and λ_z by comparing the four matrix elements of the left and right side, we get

$$\frac{d}{dt} \begin{pmatrix} \lambda_x \\ \lambda_y \\ \lambda_z \end{pmatrix} = \frac{1}{\hbar} \begin{pmatrix} 0 & -(H_{11} - H_{22}) & 2\text{Im} H_{12} \\ H_{11} - H_{22} & 0 & 2\text{Re} H_{12} \\ -2\text{Im} H_{12} & -2\text{Re} H_{12} & 0 \end{pmatrix} \times \begin{pmatrix} \lambda_x \\ \lambda_y \\ \lambda_z \end{pmatrix}.$$

The time derivative of the coherence vector $\vec{\lambda}$ can be expressed as the vector product of a 3-D vector

$$\vec{\Gamma} = \frac{1}{\hbar} \begin{pmatrix} -2\text{Re} H_{12} \\ 2\text{Im} H_{12} \\ H_{11} - H_{22} \end{pmatrix} \quad (19)$$

called Hamiltonian vector, and $\vec{\lambda}$ itself

$$\frac{d}{dt} \vec{\lambda} = \vec{\Gamma} \times \vec{\lambda}. \quad (20)$$

Note that (17) follows immediately from (20), because

$$\frac{d}{dt} (\vec{\lambda}^2) = 2\vec{\lambda} \frac{d\vec{\lambda}}{dt} = 2\vec{\lambda}(\vec{\Gamma} \times \vec{\lambda}) = 0.$$

The fully polarized $P = +1$ state corresponds to $\vec{\lambda} = (0, 0, -1)$ and the $P = -1$ state to $\vec{\lambda} = (0, 0, +1)$.

The Hamiltonian for molecule k is now represented by a Hamiltonian vector in three dimensions

$$\vec{\Gamma}^{(k)} = \left(\frac{1}{\hbar} \right) (2\gamma, 0, -\overline{P}^{(k)} E^{(k)}). \quad (21)$$

V. MODELING THE DISSIPATION OF THE ARRAY

In order to simulate the dissipation we introduce models based on the SU(2) damped Bloch equations describing the quantum dynamics of open two-state systems [7].

In the coherence vector formalism, the effect of two types of small losses, which ensures the relaxation to the ground states, and also the phase-randomizing which results in a depolarizing process associated with the contact to the environment can be built into the model [8], [9]

$$\frac{\partial \vec{\lambda}^{(k)}}{\partial t} = \vec{\Gamma}^{(k)} \times \vec{\lambda}^{(k)} - \frac{\vec{\lambda}^{(k)}}{\tau_\varphi} - \frac{\vec{\lambda}^{(k)} + \vec{\Gamma}^{(k)}}{\tau_{\text{in}}} \quad (22)$$

where τ_φ is the quantum mechanical depolarizing time associated with the contact to the environment and τ_{in} is the inelastic (dissipative) relaxation time. The environment here includes everything but the other molecules in the array, whose interactions are included explicitly. The polarization of the molecule (k) is given by $P_k = -[\vec{\lambda}^{(k)}]_z$. If we neglect the interaction with the environment ($\tau_\varphi \rightarrow \infty, \tau_{\text{in}} \rightarrow \infty$) then the length of $\vec{\lambda}_k$ equals to unity and is a constant of motion.

If $\vec{\Gamma}^{(k)}$ is constant in time and there are no losses, $\vec{\lambda}^{(k)}$ precesses about $\vec{\Gamma}^{(k)}$ with a constant angular velocity

$$\omega^{(k)} = \left| \vec{\Gamma}^{(k)} \right|. \quad (23)$$

The thermal fluctuations of the environment causes phase-randomizing, which destroys polarization and drives $\vec{\lambda}^{(k)}$ toward $\vec{\lambda}^{(k)} = 0$. The dissipation to the environment adsorbs excess energy and drives $\vec{\lambda}^{(k)}$ toward $(-\vec{\Gamma}^{(k)}/|\vec{\Gamma}^{(k)}|)$, i.e., toward the ground state.

The energy of a molecule changes in time according to

$$E^{(k)} = \frac{1}{2} \hbar \vec{\lambda}^{(k)} \vec{\Gamma}^{(k)}. \quad (24)$$

In ground state $E_0^{(k)} = (1/2)\hbar|\vec{\Gamma}^{(k)}|$, and the role of thermal fluctuations can be characterized by a temperature ratio

$$\Delta^{(k)} = \frac{E_0^{(k)}}{k_B T} \quad (25)$$

where k_B is the Boltzmann constant and T is the temperature.

It has been shown [10] that the dynamics of a molecule can be given by the state equation

$$\frac{d\vec{\lambda}^{(k)}}{dt} = \vec{\Gamma}^{(k)} \times \vec{\lambda}^{(k)} - \frac{1}{\tau_{\text{in}}} \left(\frac{1}{\tanh \Delta^{(k)}} \vec{\lambda}^{(k)} + \frac{\vec{\Gamma}^{(k)}}{|\vec{\Gamma}^{(k)}|} \right). \quad (26)$$

The coherence vector in the ground steady state

$$\vec{\lambda}^{(k)}_0 = -\frac{\vec{\Gamma}^{(k)}}{|\vec{\Gamma}^{(k)}|} \cdot \tanh \Delta^{(k)}. \quad (27)$$

Note that $\vec{\lambda}^{(k)}_0$ is an equilibrium state because $(d/dt)\vec{\lambda}^{(k)}_0 = 0$.

If molecule k is coupled to all molecules in a specified neighborhood, then in

$$\hbar \vec{\Gamma}^{(k)} = \begin{pmatrix} 2\gamma \\ 0 \\ -\sum_{\substack{j \neq k \\ j \in S^{(k)}}} E(k, j) \lambda_z^{(j)} \end{pmatrix} \quad (28)$$

the sum of the product of exchange energies $E(k, j)$ and polarization $[\lambda_z^{(j)}]$ should be extended to all neighbors in the specified neighborhood.

VI. QCA LOGIC GATES

The two-state models are in good agreement with the quantitative studies of the extended Hubbard type models, but being much simpler, there is a hope that they can be used successfully in the network design of integrated systems.

First, let us study the interactions between two molecules, each consisting of four dots and each occupied by two electrons. The electrons are allowed to tunnel between the dots in the same molecule, but not between different molecules. Since the tunneling probabilities decay exponentially with distance, this can be achieved by having a larger dot-dot distance between cells,

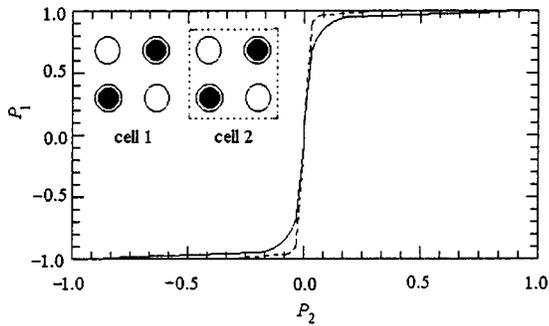


Fig. 2. Molecule-molecule coupling.

than within the same cell. Coupling between the two cells is provided by the Coulomb interaction between the electrons in different cells.

Fig. 2 shows how one molecule is influenced by the state of its neighbor. The inset shows two molecules where the polarization of molecule 1 (P_1) is determined by the polarization of its neighbor (P_2). The polarization of molecule 2 is presumed to be fixed at a given value, corresponding to a certain arrangement of charges in molecule 2, and this charge distribution exerts its influence on molecule 1, thus determining its polarization P_1 . The important finding here is the strongly nonlinear nature of the molecule-molecule coupling. As shown in the figure, molecule 1 is almost completely polarized even though molecule 2 might only be partially polarized. For example, a polarization of $P_2 = 0.1$ induces almost perfect polarization in molecule 1, i.e., $P_1 = 0.99$. In other words, even a small asymmetry of charge in molecule 2 is sufficient to break the degeneracy of the two basic states in molecule 1 by energetically favoring one configuration over the other.

The abruptness of the molecule-molecule response function depends upon the ratio of the strength of the tunneling energy to the Coulomb energy for electrons on neighboring sites. This reflects a competition between the kinetic and potential energy of the electron. For a large tunneling energy, an electron has a tendency to spread out more evenly over the available dots, and the nonlinearity becomes less pronounced. Stronger Coulomb coupling tends to keep electrons apart, and the nonlinearity becomes more pronounced. Properly designed molecules will possess strongly nonlinear coupling characteristics.

Next, we will show that the physical interactions between molecules may be used to realize elementary Boolean logic functions [11]–[13].

Fig. 3 shows examples of simple molecular arrays. In each case, the polarization of the molecule at the edge of the array is kept fixed; this is the so-called driver molecule and it is plotted with a thick border. We call it the driver since it determines the state of the whole array. Without a polarized driver, the molecules in a given array would be unpolarized in the absence of a symmetry-breaking influence that would favor one of the basis states over the other. Each figure shows the molecular polarization corresponding to the physical ground state configuration of the whole array.

Fig. 3(a) shows that a line of molecules allows the propagation of information, thus realizing a binary wire. Note that only polarization (charge configuration encoding information), but

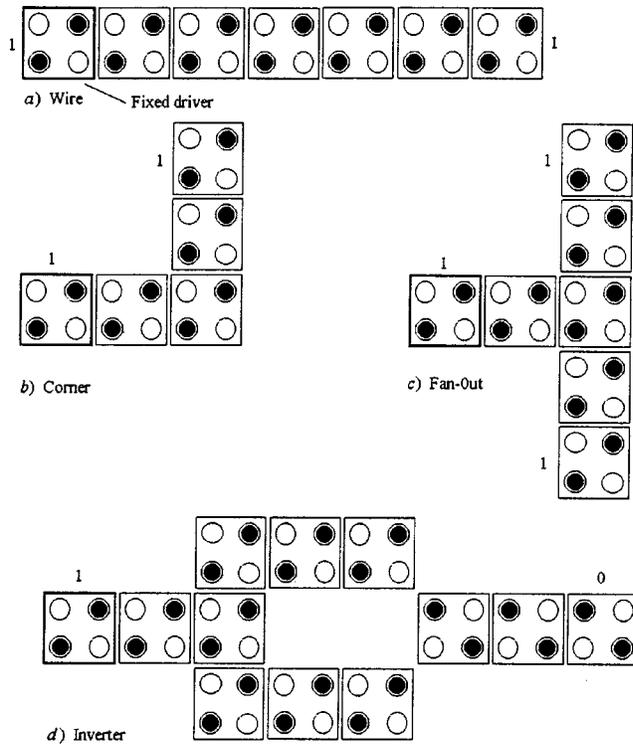


Fig. 3. Molecular arrays realizing elementary logic functions: (a) wire, (b) corner, (c) fan-out, and (d) inverter.

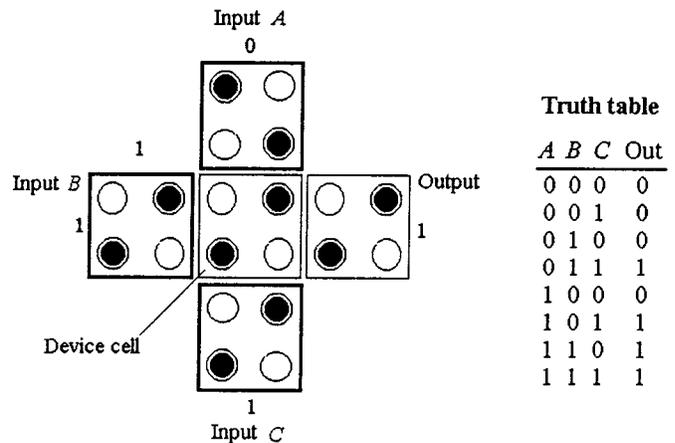


Fig. 4. Majority logic gate.

no electric current flows down the line. Information can also flow around corners, as shown in Fig. 3(b), and fan-out is possible, compare Fig. 3(c). A specific arrangement of cells, such as the one shown in Fig. 3(d), may be used to realize an inverter.

These quantum-dot networks, or “artificial molecular arrays” are examples of quantum-functional devices. Utilizing quantum-mechanical effects for device operation may give rise to new functionality. Fig. 4 shows a majority logic gate, which simply consists of an intersection of lines and the “device molecule” is just the one in the center. If we view three of the neighbors as inputs (kept fixed), then the polarization of the output cell is the one which “computes” the majority votes of the inputs. The figure also shows the majority logic truth table which was computed as the physical ground state polarization for a given combination of inputs.

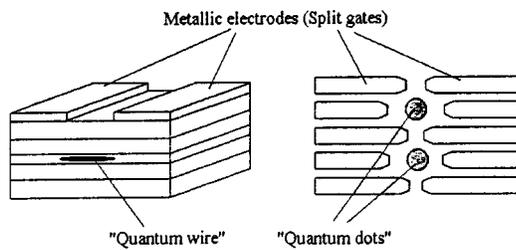


Fig. 5. Quantum wire and quantum dot confined by electrostatic split gates.

Note that conventional AND and OR gates are hidden in the majority logic gate. Inspection of the majority-logic truth table reveals that if input A is kept fixed at 0, the remaining two inputs B and C realize an AND gate. Conversely, if A is held at 1, inputs B and C realize a binary OR gate. In other words, majority logic gates may be viewed as programmable AND and OR gates.

Figs. 5 and 6 illustrates some of the possible realizations of QCA molecules. In Fig. 5, the electrostatic split gates are shown resulting in “wire”-like and “dot”-like quantum confinement [14], [15].

Fig. 6 illustrates the three possibilities of the realization of a QCA molecule:

- 1) the semiconductor quantum dot cell;
- 2) the metal-island QCA;
- 3) molecular QCA.

The fabrication of QCA cell by split-gate technology is a challenging problem, yet appears to be within reach of current lithographic capability. Fig. 5 shows a possible physical realization which is based on electrostatic confinement provided by a top metallic electrode.

In addition to the semiconductor systems single-electron tunneling phenomena may also be observed in metallic tunnel junctions. Consider a ring of metallic tunnel junctions, schematically shown in Fig. 6(b). The tunnel junctions are represented by the crossed capacitor symbols, indicating that these junctions are characterized by capacitance and tunnel resistance. The metallic droplets themselves are the “wires” between these tunnel junctions. Consider now that two extra electrons are added to such cell, as schematically shown in the figure. It has been shown that this cell exhibits precisely the same two distinct ground state configurations as the semiconductor cell. In addition, the cell–cell coupling also shows the same strongly nonlinear saturating characteristic. The first experimental implementation of a QCA-type majority gate has been demonstrated by rings of metallic tunnel junctions [21].

QCA room temperature operation would require molecular-scale implementations of the basic cell. Molecular chemistry promises to offer the versatility for the desired miniaturization. A candidate for such a prototypical molecular cell has been synthesized and crystallographically characterized [25]. As schematically illustrated in Fig. 6(c), these molecular substances with the formula $M_2\{(CO)_9Co_3CC\}_2$, where $M = Mo, Mn, Fe, Co, Cu$, consist of square arrays of transition metal clusters: each containing three cobalt atoms. It is remarkable that the four clusters are arranged in a (flat) square, as opposed to a (3-D) tetrahedron. Each cell has an edge-to-edge distance of

about 2 nm, which is precisely the desired dimension for QCA room temperature operation.

VII. THE ROLE OF DEVICE-ACTIVITY IN SIGNAL PROCESSING

The signal processing potential of nonlinear networks has been recently explored with the fundamental conclusion that local-activity of the cells is necessary to exhibit complexity [2]. To write, store, transform, transmit and to read information, i.e., to process signals in a broad sense can not be performed without exhibiting complexity, thus local activity is a necessary condition of signal processing as well.

The *sine qua non* of information processing is 1) the ability to achieve *signal-power-gain* and 2) to have units with *multiple equilibria*. Until now, both have been based on *active devices* with the ability to transform power from an *energy source* into the *signal-flow*.

The role of the energy source is played by *direct-current power supplies* in case of vacuum-tube and transistor amplifiers, by *time-varying pumps* in case of masers, lasers, and also in case of low noise varactor amplifiers of radio astronomy. The clock signals in computing are fulfilling this role as well. The molecular signal processors in plants performing photosynthesis are pumped by solar energy, and the molecular processors in animals are fueled by the energy of metabolism.

The 50 glorious years of the solid-state transistor demonstrates how a three-terminal tiny device on a silicon chip can efficiently transform the chemical energy stored in a battery into signal-energy, and by achieving this to become a universal active device of the information technology. In the transistor the chemical energy of a battery is transformed into kinetic energy of the majority and minority carriers, then the signal perturbing the flow of the minority carriers controls the flow of the majority carriers and this results in significant power-gain, because quantum-statistics insures that the product of majority and minority carrier concentrations is constant. The transistor is a *active device par excellence*, and the workhorse of microelectronics.

Why is device activity necessary for signal processing? In case of the amplifiers with signal-power gain the answer is self-evident. But is device activity a necessary property of computing as well? Is it not possible to build a computer from passive devices, e.g., just from switches?

The model of the simplest binary processor consists of two parts; a tape (memory) and a finite-state machine, which moves over the tape, reads its content and writes on it. Indeed, no processor exists without devices capable of storing bits, which can be written-in, held, read, and rewritten again.

The simplest model of a single-bit memory cell is a device having two well distinguishable physical states, one of them assigned to logic value “1,” the other to logic value “0.” We want the device to hold its state until we decide to reset it. Thus, the simplest memory cell should have two inputs. If both inputs stay in state “0,” the device should hold its value, thus it can be in “0” or in “1.” Thus, in this device, for the same boundary values two different equilibrium states should hold: “0” and “1,” thus it is necessary to have devices with two distinguishable equilibria.

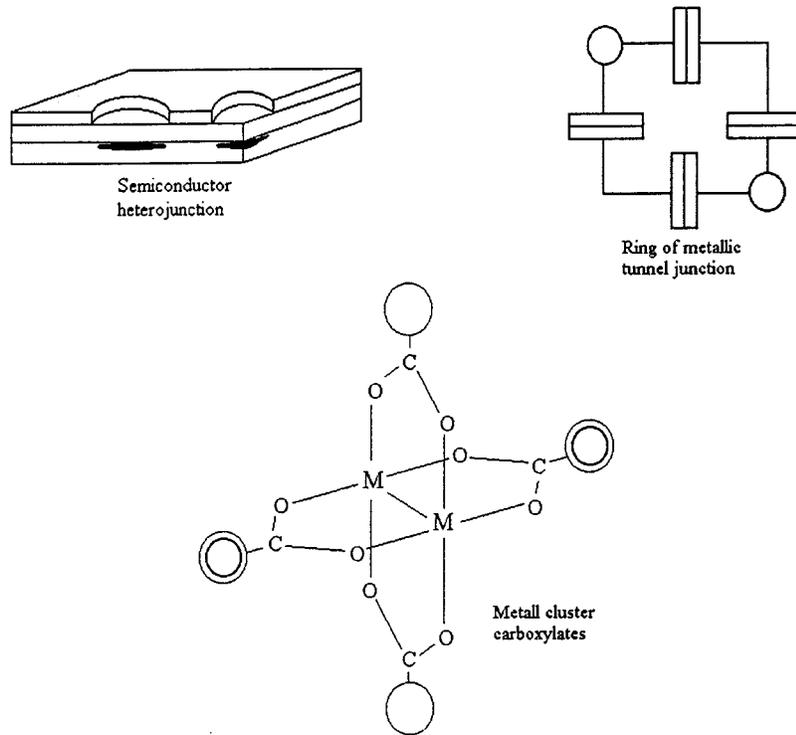


Fig. 6. QCA molecule realized by (a) semiconductor quantum dot cell, (b) metal islands, and (c) carboxylates molecule.

The existence and uniqueness of equilibrium states of networks composed of linear and nonlinear devices have been studied [16]. It has been shown that n -port networks with state $\mathbf{x}(t)$, port currents $\mathbf{i}(t)$, and port voltages $\mathbf{v}(t)$, which are described by nonlinear dynamic equations (Fig. 7)

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}[\mathbf{x}(t), \mathbf{i}(t)]; \quad \mathbf{v}(t) = \mathbf{g}[\mathbf{x}(t), \mathbf{i}(t)] \quad (29)$$

the local dynamics around existing equilibrium points provide information about the global behavior of the network as a whole. The equilibrium points are defined by

$$\mathbf{i}(t) = \mathbf{I}_0, \quad \left. \frac{d\mathbf{x}(t)}{dt} \right|_{\mathbf{i}=\mathbf{I}_0} = \mathbf{0} \Rightarrow \mathbf{x}_0, \mathbf{v}_0. \quad (30)$$

Note that in microelectronics this equilibrium is built up by a direct current (dc) power supply. If no signal dynamics takes place, the network is assumed to stay in its equilibrium state. When a small signal is switched on, the direction of the dynamics depends on the perturbation of the state equations around the equilibrium point, in which the network stayed before the signal input.

If we introduce infinitesimal perturbations and neglect the higher order terms of perturbing $\Delta v_k(t)$ voltages and $\Delta i_k(t)$ currents, we obtain a set of linearized state equations, the so called *local state equation at an equilibrium point*. The relation between these n -port currents and voltages is linear.

The signal power flow corresponding to the given perturbing signals (boundary conditions) around the equilibrium state, subject to zero initial states, can be given as

$$p(t) = \sum_{k=1}^n \Delta v_k(t) \cdot \Delta i_k(t), \quad t \geq 0. \quad (31)$$

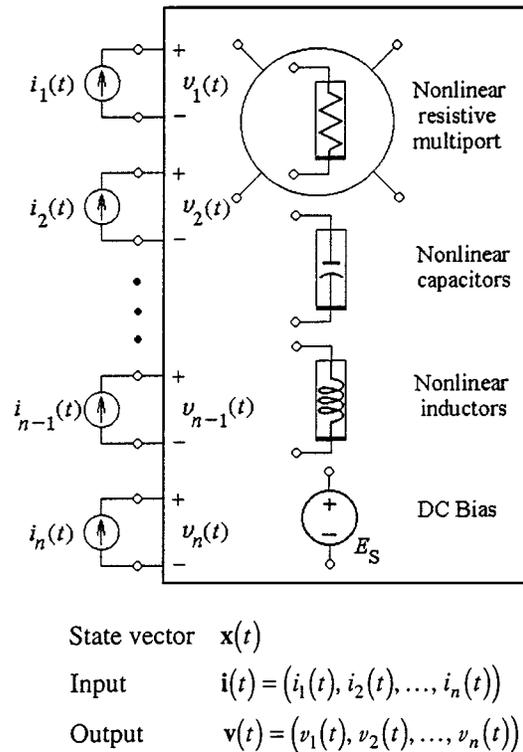


Fig. 7. Nonlinear dynamic n -port.

The local power flow at time t at the equilibrium point is the instantaneous signal power flowing into the network. If $p(t)$ is negative then power flows from the network into the signal sources. The sign of the local power flow can change in time, but

for passive devices and passive networks, the integrated local power flow is positive

$$\int_0^T p(t) dt \geq 0 \quad (32)$$

for any $T > 0$, i.e., the network cannot deliver more energy than the amount it had absorbed before. A device or a network of devices is called *locally passive* if at every equilibrium point (32) holds, and it is called *locally active* if there is at least one equilibrium point at which it is *not passive*. Note that diodes or switches are examples of locally passive nonlinear resistors.

It has been shown that networks composed of locally passive devices are locally passive, i.e., local passivity is a closure property, and the network of Fig. 7 has a *unique and asymptotically stable equilibrium point* if all devices (nonlinear resistors, capacitors, and inductors) are *locally passive*, and there is no loop formed exclusively by capacitors, or no cut-set exclusively formed by inductors. Thus, a network composed of locally passive devices can not have multiple equilibria.

Without the ability to transform power from an *energy source* into the *signal flow*, i.e., by applying exclusively locally passive devices and time-invariant energy sources (dc power supplies), we cannot achieve 1) *signal-power gain* and/or 2) *controllable multiple equilibria*. Thus local activity is a *necessary condition* of the realizability of 1) *amplifiers* and/or 2) *read, hold, and write memory cells*.

We have seen that local activity is a property of a linear system, namely, of a linear n -port. There exist many equivalent passivity criteria in the literature for testing the passivity of linear n -ports. The criteria are given as necessary and sufficient conditions on the impedance, admittance or scattering operators of the linear n -port. These operators relate the Laplace-transform of the port voltages and currents, or the incident and reflected waves, thus they are represented by matrices whose elements are functions of a complex variable s .

$$\left. \begin{aligned} \mathbf{V}(s) &\triangleq \int_0^\infty \Delta \mathbf{v}(t) e^{-st} dt \\ \mathbf{I}(s) &\triangleq \int_0^\infty \Delta \mathbf{i}(t) e^{-st} dt \end{aligned} \right\} \quad (33)$$

$$\left. \begin{aligned} \mathbf{V}(s) &= \mathbf{Z}(s) \cdot \mathbf{I}(s) \\ \mathbf{I}(s) &= \mathbf{Y}(s) \cdot \mathbf{V}(s) \end{aligned} \right\}. \quad (34)$$

A matrix as a function of the complex variable s is the impedance (or admittance) matrix of a linear passive N -port if and only if it is *positive real* (PR), or equivalently it is the scattering matrix of the n -port if and only if the matrix is *bounded real* (BR) [17]. A matrix is positive real (PR) if and only if the following four conditions are met:

- 1) on the open right half plane of s the matrix has no poles;
- 2) along the imaginary axes of s the matrix plus its conjugate transpose is positive semidefinite;
- 3) the matrix does not have multiple poles on the imaginary axes;
- 4) at simple poles on the imaginary axes the associated residue matrix is a positive semidefinite Hermitian matrix. If any one of the four criteria of positive reality is not met, the n -port is *locally active*.

VIII. GROUND-STATE MOLECULES ARE LOCALLY PASSIVE

A. A “Driver” and a Driven Molecule

In order to build an analogy between the voltage–current relationship of n -ports and the coherence-vectors of two-state molecules, let us first have a look at a pair of two coupled molecules. Let us assume that both are in equilibrium states $\vec{\lambda}_0^{(1)}$ and $\vec{\lambda}_0^{(2)}$. Thus, the polarizations $\lambda_{z0}^{(1)}$ and $\lambda_{z0}^{(2)}$ are also fixed, i.e., $\vec{\Gamma}^{(1)} = \vec{\Gamma}_0^{(1)}$ and $\vec{\Gamma}^{(2)} = \vec{\Gamma}_0^{(2)}$ at equilibrium.

In equilibrium state $(d\vec{\lambda}^{(2)}/dt) = 0$. In case of small losses, (26) in equilibrium reads for $\vec{\lambda}_0^{(2)}$

$$\frac{d\vec{\lambda}_0^{(2)}}{dt} = \vec{\Gamma}_0^{(2)} \times \vec{\lambda}_0^{(2)} - \frac{1}{\tau_{\text{in}} \tanh \Delta} \vec{\lambda}_0^{(2)} - \frac{1}{\tau_{\text{in}}} \frac{\vec{\Gamma}_0^{(2)}}{|\vec{\Gamma}_0^{(2)}|} = 0. \quad (35)$$

To solve (35) in a matrix form let us simplify the notations for the constants, such as

$$a = \frac{1}{\tanh \Delta}, \quad b = \frac{E_{12}}{\hbar}, \quad c = \frac{2\gamma}{\hbar}. \quad (36)$$

Equation (35) in matrix form

$$\begin{pmatrix} -\frac{a}{\tau_{\text{in}}} & b\lambda_{z0}^{(1)} & 0 \\ -b\lambda_{z0}^{(1)} & -\frac{a}{\tau_{\text{in}}} & -c \\ 0 & c & -\frac{a}{\tau_{\text{in}}} \end{pmatrix} \begin{pmatrix} \lambda_{z0}^{(1)} \\ \lambda_{y0}^{(1)} \\ \lambda_{z0}^{(1)} \end{pmatrix} - \frac{1}{\tau_{\text{in}}} \frac{1}{\sqrt{\left(\frac{c}{b}\right)^2 + \left(\lambda_{z0}^{(1)}\right)^2}} \begin{pmatrix} \frac{c}{b} \\ 0 \\ -\lambda_{z0}^{(1)} \end{pmatrix} = 0. \quad (37)$$

Equation (37) has a unique solution, because the matrix to be inverted is not singular. Solving (37), we get

$$\begin{aligned} \vec{\lambda}_0^{(2)} &= \frac{1}{a\sqrt{\left(\frac{c}{b}\right)^2 + \left(\lambda_{z0}^{(1)}\right)^2}} \begin{pmatrix} \frac{c}{b} \\ 0 \\ -\lambda_{z0}^{(1)} \end{pmatrix} \\ &= -(\tanh \Delta) \frac{\vec{\Gamma}_0^{(2)}}{|\vec{\Gamma}_0^{(2)}|}. \end{aligned} \quad (38)$$

The energy content of molecule (2) according to (24)

$$E^{(k)} = \frac{1}{2} \hbar \vec{\lambda}^{(2)} \vec{\Gamma}^{(2)}. \quad (39)$$

At equilibrium the energy of the molecule

$$E = \frac{1}{2} \hbar \vec{\lambda}_0^{(2)} \vec{\Gamma}_0^{(2)} = -\frac{1}{2} \hbar \frac{1}{a} \left| \vec{\Gamma}_0^{(2)} \right| \quad (40)$$

or in our single-driver case

$$E_0 = -\frac{1}{2} \frac{b}{a} \sqrt{\left(\frac{c}{b}\right)^2 + \left(\lambda_{z0}^{(1)}\right)^2}. \quad (41)$$

Let us assign to molecule (2) formal “charge” and “voltage” vectors

$$\vec{q}^{(2)} \triangleq e\vec{\lambda}^{(2)}, \quad \vec{v}^{(2)} \triangleq \frac{\hbar}{e} \vec{\Gamma}^{(2)} \quad (42)$$

where $e = 1.6022 \cdot 10^{-19}$ As is the value of the electrons' charge, and $\hbar = 1.0546 \cdot 10^{-34}$ VAs² is the Planck's constant per 2π . The energy of molecule (2) can be expressed by $\vec{q}^{(2)}$ and $\vec{v}^{(2)}$: $E = (1/2)\vec{q}^{(2)} \cdot \vec{v}^{(2)}$.

We have two coupled molecules. Molecule (1) is the "driver," molecule (2) is "driven." This means that we force $\lambda_z^{(1)}$ as a function of time about its equilibrium state

$$\lambda_z^{(1)} = \lambda_{z0}^{(1)} + \Delta\lambda_z^{(1)}(t) \quad (43)$$

i.e., $\Delta\lambda_z^{(1)}(t)$ is given. This means that through (42) molecule (1) determines the voltage vector of molecule (2). Note that molecule (2) is driven only through its "z"-port, thus looking at molecule (2) from molecule (1), it is a one-port, driven by $\vec{v}_z^{(2)}$.

In this single-driver and single-driven molecule case, molecule (2) is a nonlinear one-port, with three state-variables, $\lambda_x^{(2)}$, $\lambda_y^{(2)}$, and $\lambda_z^{(2)}$ driven by a voltage source.

Let us follow Chua's procedure in checking the local properties of the one-port in the neighborhood of the equilibrium point. We linearize the state equation (26) in the neighborhood of $\vec{\lambda}_0^{(2)}$. We have to take into account the perturbation of $\vec{\Gamma}^{(2)}$ as well, because $\vec{\Gamma}$ depends on the neighbor's polarization. Thus, $\vec{\lambda}^{(1)} = \vec{\lambda}_0^{(1)} + \Delta\vec{\lambda}^{(1)}$, and $\vec{\lambda}^{(2)} = \vec{\lambda}_0^{(2)} + \Delta\vec{\lambda}^{(2)}$, $\vec{\Gamma}^{(2)} = \vec{\Gamma}_0^{(2)} + \Delta\vec{\Gamma}^{(2)}$. Substituting the perturbed vectors into (26) we get

$$\begin{aligned} \frac{d\Delta\vec{\lambda}^{(2)}}{dt} &= \vec{\Gamma}_0^{(2)} \times \Delta\vec{\lambda}^{(2)} + \Delta\vec{\Gamma}^{(2)} \times \vec{\lambda}_0^{(2)} \\ &\quad - \frac{1}{\tau} \left[a\vec{\lambda}_0^{(2)} + a\Delta\vec{\lambda}^{(2)} + \frac{\vec{\Gamma}_0^{(2)}}{|\vec{\Gamma}_0^{(2)}|} \right. \\ &\quad \left. + \left(\frac{\vec{\Gamma}^{(2)}}{|\vec{\Gamma}^{(2)}|} - \frac{\vec{\Gamma}_0^{(2)}}{|\vec{\Gamma}_0^{(2)}|} \right) \right]. \end{aligned} \quad (44)$$

Note that we recognized $\vec{\Gamma}_0^{(2)} \times \vec{\lambda}_0^{(2)} = 0$, and $\Delta\vec{\Gamma}^{(2)} \times \Delta\vec{\lambda}^{(2)}$ is negligible. In (44)

$$a\vec{\lambda}_0^{(2)} + \frac{\vec{\Gamma}_0^{(2)}}{|\vec{\Gamma}_0^{(2)}|} = 0 \quad (45)$$

because $\vec{\lambda}_0^{(2)}$ is an equilibrium coherence vector

$$\vec{\Gamma}_0^{(2)} \times \Delta\vec{\lambda}^{(2)} = \begin{pmatrix} 0 & b\lambda_{z0}^{(1)} & 0 \\ -b\lambda_{z0}^{(1)} & 0 & -c \\ 0 & c & 0 \end{pmatrix} \begin{pmatrix} \Delta\lambda_x^{(2)} \\ \Delta\lambda_y^{(2)} \\ \Delta\lambda_z^{(2)} \end{pmatrix} \quad (46)$$

$$\Delta\vec{\Gamma}^{(2)} \times \vec{\lambda}_0^{(2)} = \frac{1}{a\sqrt{\left(\frac{c}{b}\right)^2 + \left(\lambda_{z0}^{(1)}\right)^2}} \begin{pmatrix} 0 \\ c\Delta\lambda_z^{(1)} \\ 0 \end{pmatrix} \quad (47)$$

and

$$\frac{\vec{\Gamma}^{(2)}}{|\vec{\Gamma}^{(2)}|} - \frac{\vec{\Gamma}_0^{(2)}}{|\vec{\Gamma}_0^{(2)}|} \quad (48)$$

is the difference between two unit vectors. Note that both of them lie in the x - z plane, thus both vectors can be characterized by an angle

$$\begin{aligned} \frac{\vec{\Gamma}^{(2)}}{|\vec{\Gamma}^{(2)}|} &= \frac{1}{\sqrt{\left(\frac{c}{a}\right)^2 + \left(\lambda_z^{(1)}\right)^2}} \begin{pmatrix} \frac{c}{b} \\ 0 \\ -\lambda_z^{(1)} \end{pmatrix} \\ &= \begin{pmatrix} \cos\varphi^{(2)} \\ 0 \\ -\sin\varphi^{(2)} \end{pmatrix} \end{aligned} \quad (49)$$

and

$$\begin{aligned} \frac{\vec{\Gamma}_0^{(2)}}{|\vec{\Gamma}_0^{(2)}|} &= \frac{1}{\sqrt{\left(\frac{c}{a}\right)^2 + \left(\lambda_{z0}^{(1)}\right)^2}} \begin{pmatrix} \frac{c}{b} \\ 0 \\ -\lambda_{z0}^{(1)} \end{pmatrix} \\ &= \begin{pmatrix} \cos\varphi_0^{(2)} \\ 0 \\ -\sin\varphi_0^{(2)} \end{pmatrix}. \end{aligned} \quad (50)$$

For small phase difference

$$\frac{\vec{\Gamma}^{(2)}}{|\vec{\Gamma}^{(2)}|} - \frac{\vec{\Gamma}_0^{(2)}}{|\vec{\Gamma}_0^{(2)}|} \approx \cos^2\varphi_0 \begin{pmatrix} \frac{b}{c} \sin\varphi_0 \\ 0 \\ \frac{b}{c} \cos\varphi_0 \end{pmatrix} \Delta\lambda_z^{(1)}. \quad (51)$$

The equilibrium $\vec{\lambda}_{z0}^{(1)}$ can be expressed by φ_0 , because $\tan\varphi_0 = (\sin\varphi_0/\cos\varphi_0) = (b/c)\lambda_{z0}^{(1)}$, thus $b\lambda_{z0}^{(1)} = c\tan\varphi_0$.

Substituting (45)–(51) into (44), we get a set of linear differential equations describing the perturbed dynamics at equilibrium. This set of local state equations can be solved for the state variables $\Delta\lambda_x^{(2)}$, $\Delta\lambda_y^{(2)}$, and $\Delta\lambda_z^{(2)}$ by applying Laplace-transform. This way we can relate the port-variables.

$$\begin{aligned} \frac{d\Delta\vec{\lambda}^{(2)}}{dt} &= \begin{pmatrix} -\frac{a}{\tau_{in}} & b\lambda_{z0}^{(1)} & 0 \\ -b\lambda_{z0}^{(1)} & -\frac{a}{\tau_{in}} & -c \\ 0 & c & -\frac{a}{\tau_{in}} \end{pmatrix} \Delta\vec{\lambda}^{(2)} \\ &\quad + \begin{pmatrix} \frac{1}{\tau_{in}} \frac{b}{c} \sin\varphi_0 \cos\varphi^2\varphi_0 \\ \frac{b}{a} \cos\varphi_0 \\ \frac{1}{\tau_{in}} \frac{b}{c} \cos\varphi_0 \cos\varphi^2\varphi_0 \end{pmatrix} \lambda_z^{(1)}. \end{aligned} \quad (52)$$

Equation (52) can be solved by Laplace-transform technique. The initial conditions for $\Delta\vec{\lambda}^{(2)}$ can be set to zero, because the perturbed dynamics starts from an equilibrium. The one-port admittance

$$Y(s) = \frac{As}{\left(s + \frac{a}{\tau}\right)^2 + \frac{c^2}{\cos^2\varphi_0}} + \frac{1}{\tau} \frac{B\left(s + \frac{a}{\tau}\right)}{\left(s + \frac{a}{\tau}\right)^2 + \frac{c^2}{\cos^2\varphi_0}} \quad (53)$$

where A and B are positive constants. When losses decrease $a \rightarrow 1$ and $\tau \rightarrow \infty$.

The admittance given by (53) is positive real (PR). (It is the admittance of two *RLC* passive circuits.) The four criteria of positive reality are clearly met.

From the positive reality of impedance (53) it follows that time-invariant two-state molecules described by state equation (26) are locally passive, thus the arrays composed of them cannot possess multiple equilibria or cannot realize signal-power-gain.

IX. SIGNAL PROCESSING WITH “TIME-VARYING” DEVICES

We have seen that systems composed of time-invariant and locally passive devices cannot process signals, because neither signal-power-gain nor multiple equilibria are achievable. However, a locally active device can transform the power of a dc supply into a time-varying power supply, which can generate sinusoidal or time-varying clock-signal like voltage.

If a strongly nonlinear locally passive device is integrated with a time-varying power generator, e.g., with a clock signal source, then for the small signals to be processed this combined circuit will behave like a device with “time-varying” parameters.

We have seen that the QCA molecule is a strongly nonlinear device. The off-diagonal Hamiltonian matrix element γ can be controlled by the voltage of a metal gate. If the value of γ is small compared to E_k , then the polarization will saturate near +1 and -1, and the response will be close to a step function. As γ is increased, both the slope and the saturation values decrease. For high enough γ , the polarization can be fixed near zero. This control can be used for adiabatic switching.

Adiabatic switching of two-state molecules described by state-equations (7) or (26) has been introduced to control the inelastic processes relaxing the molecule to its ground state [9]. To avoid undesirable metastable traps during the desirable relaxation to the true ground state a mode of switching was introduced in which the QCA always remains in its instantaneous ground state. The quantum mechanical adiabatic theorem states that if the Hamiltonian of a system undergoes a gradual (sufficiently slow) change from an initial to a final form, and if a particle starts in the n th nondegenerate eigenstate of the initial Hamiltonian, it will be carried under the time-dependent Schrödinger equation into the n th eigenstate of the final Hamiltonian.

If the interdot barriers, i.e., the parameter γ in the state equation (26) can be controlled from outside, the molecules can be switched adiabatically by lowering the interdot barriers within the molecule and switching the input signal, followed by raising the barriers. The theorem guarantees that the system, which starts in the ground state of the initial Hamiltonian, will be carried smoothly into the ground state of the new Hamiltonian. Fig. 8 shows a schematic diagram of the adiabatic switching. The system begins in the ground state appropriate to an old input. Lowering the interdot barriers reduces the confinement of the electrons on the individual quantum dots, while removal of the old input removes the external boundary condition that was driving the system into one of the polarization states. The two-electron wavefunctions become delocalized across the molecule. Next, the new inputs are being applied and the interdot

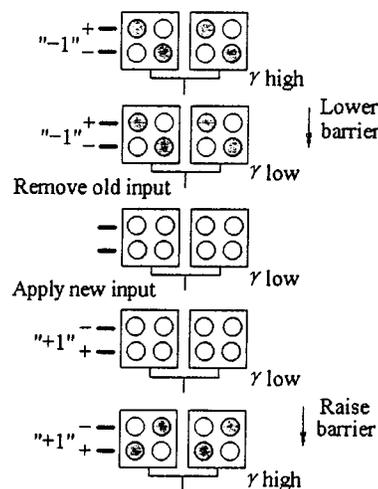


Fig. 8. Adiabatic switching.

barriers are raised, thus the electrons become localized and the molecules are driven into the polarization state corresponding to the new input.

The very same adiabatic control mechanism of molecules can be introduced to realize molecules with slowly (adiabatically) time-varying interdot barriers, i.e., with time-varying γ parameters. The energy dissipated to the environment will be restored by power flowing from the control electrodes into the molecules.

Using time-varying control of γ addressable memory units can be constructed. Fig. 9 illustrates the molecular array which realizes an SR flip-flop with the help of a four-phase clock-control [18].

Let us assume that at the beginning of a clock period the state of Q is either “0” or “1.” Clocks #4 and #3 are down, i.e., all the molecules controlled by them are in the same state as Q . If $S = R = “0,”$ the output of majority gate (NOT R , “0,” Q) results in Q , and $(S, “1,” Q)$ is also Q . Thus the molecules controlled by clock #2 are also in state Q . We lower clock signals #1 and #2 and then set or reset the flip-flop. If we set $S = “1,”$ then independently of the value Q , the output of majority gate $(S, “1,” Q)$ becomes “1,” which through the molecules controlled by clock #2, #3 and finally #4 set every molecule, including Q into $Q = “1.”$ If instead of setting S , we reset $R = “1,”$ then the output of majority gate (NOT R , “0,” Q) will become “0,” which sets the output of the $(S, “1,” Q)$ to “0,” thus Q will become “0.”

It is envisaged that a rich variety of time-varying molecular networks can be realized by multiphase adiabatic clock signals. Subarrays of molecules could be connected to each clock signal, and a multiphase adiabatic clocking scheme could control the signal flow. It can be shown that a four-phase clock can provide a time-varying environment for addressable memory and programmable logic arrays, thus for general purpose computing.

The lack of local activity in artificial molecules and the geometrical difficulties of the adiabatic clock control (high-density wiring) call for a new approach which combines locally passive quantum dot-arrays with locally active resonant-tunneling devices and field-effect transistors. Clock signals cannot be generated but with the help of transistors. The interface between

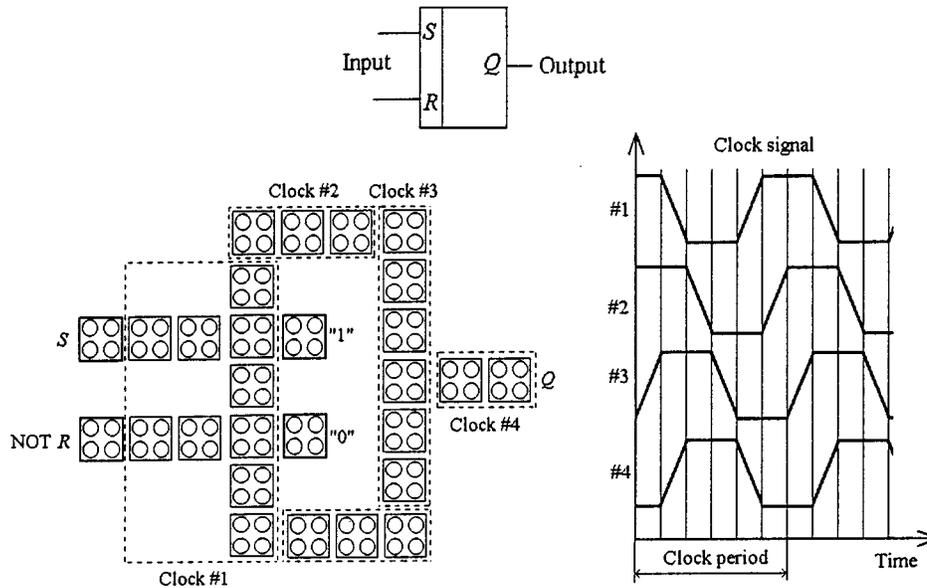


Fig. 9. (a) Single-bit memory: SR flip-flop. (b) SR flip-flop realized by four-phase clocked QCA.

the molecular processing units and the environment could only be realized by transistors as well. Thus, the first generation of nanoelectronic chips will most probably be built as a combined network of time-varying (i.e., clock controlled) quantum-dot arrays, resonant tunneling devices, and field-effect transistors.

In principle, universal digital processors could be constructed and built from adiabatically controlled two-state molecules alone. However, the challenges of integration, the formidable difficulties of wiring the adiabatic control on a chip of large complexity calls for locally connected cellular architectures. The paradigm of cellular-nonlinear-network universal machines (CNN-UM) [19] provide a natural architectural concept for nanoelectronic signal processing. It is envisaged that a robust nanoelectronic CNN-UM cell itself could only be realized by a circuit composed not only of adiabatically controlled molecules, but transistors as well. The more functions are solved by molecules, the smaller, the faster, and lower power the chip could be.

ACKNOWLEDGMENT

The authors are grateful to L. O. Chua, G. I. Iafrate, S. Goodnick, Y.-F. Huang, R.-W. Liu, J. Nossek and T. Roska for stimulating discussions.

REFERENCES

- C. S. Lent, P. D. Tougaw, W. Porod, and G. H. Bernstein, "Quantum cellular automata," *Nanotechnology*, vol. 4, pp. 49–57, 1993.
- L. O. Chua, *CNN: A Paradigm for Complexity*, Singapore: World Scientific, 1998.
- G. J. Iafrate and M. A. Strosio, "Application of quantum-based devices: Trends and challenges," *IEEE Trans. Electron Devices*, vol. 43, pp. 1621–1625, Oct. 1996.
- Á. I. Csurgay, "The circuit paradigm in nanoelectronics," in *Proc. Eur. Conf. Circuit Theory Design, ECCTD'97*, Budapest, Hungary, 1997, pp. 240–246.
- P. D. Tougaw, C. S. Lent, and W. Porod, "Bistable saturation in coupled quantum-dot cells," *J. Appl. Phys.*, vol. 74, pp. 3556–3558, 1993.
- G. Tóth, C. S. Lent, P. D. Tougaw, Y. Brazhnik, W. Weng, W. Porod, R.-W. Liu, and Y.-F. Huang, "Quantum cellular neural networks," *Superlatt. Microstructures*, vol. 20, pp. 473–477, 1996.
- G. Mahler and V. A. Weberruss, *Quantum Networks—Dynamics of Open Nanostructures*. Berlin, Germany: Springer-Verlag, 1995.
- C. S. Lent, "Dynamics of quantum-dot cellular automata and cellular nonlinear networks," in *Proc. Eur. Conf. Circuit Theory Design, ECCTD'97*, Budapest, Hungary, 1997, pp. 254–258.
- C. S. Lent and P. D. Tougaw, "A device architecture for computing with quantum-dots," *Proc. IEEE*, vol. 85, pp. 541–547, Apr. 1997.
- C. S. Lent and J. Timler, . unpublished.
- P. D. Tougaw and C. S. Lent, "Logical devices implemented using quantum cellular automata," *J. Appl. Phys.*, vol. 75, pp. 1818–1825, 1994.
- W. Porod, "Quantum-dot devices and quantum-dot cellular automata," *Int. J. Bifurcation Chaos*, vol. 7, no. 11, 1997.
- W. Porod, C. S. Lent, G. Tóth, H. Luo, Á. I. Csurgay, Y.-F. Huang, and R.-W. Liu, "Quantum-dot cellular nonlinear networks: Computing with locally-connected quantum-dot arrays," in *Proc. IEEE Int. Symp. Circuits Systems, ISCAS'99*, Hong Kong, June 1999.
- M. Chen and W. Porod, "Design of gate-confined quantum-dot structures in the few-electron regime," *J. Appl. Phys.*, vol. 78, pp. 1050–1057, 1995.
- W. Porod, C. S. Lent, G. H. Bernstein, A. O. Orlov, I. Amlani, G. L. Sneider, and J. L. Merz, "Quantum-dot cellular automata: Computing with coupled quantum dots," *Int. J. Electron.*, vol. 86, no. 5, pp. 549–590, 1999.
- L. O. Chua, "Device modeling via basic nonlinear circuit elements," *IEEE Trans. Circuits Syst.*, vol. 27, pp. 1014–1044, Nov. 1980.
- H. J. Carlin and P. P. Civalleri, *Wideband Circuit Design*. Boca Raton, FL: CRC, 1998.
- G. Tóth, . unpublished.
- L. O. Chua and T. Roska, "The CNN paradigm," *IEEE Trans. Circuits Syst.*, vol. 40, no. 3, pp. 147–156, Mar. 1993.
- S. Goodnick, W. Porod, Á. I. Csurgay, C. Gerousis, X. Wang, G. Tóth, and C. S. Lent, "Modeling nanoelectronic CNN cells: CMOS, SET's and QCAs," in *Proc. Euro. Conf. Circuit Theory Design, ECCTD'99*, Stresa, 1999.
- I. Amlani, A. O. Orlov, G. Tóth, G. H. Bernstein, C. S. Lent, and G. L. Sneider, "Digital logic gate using quantum-dot cellular automata," *Science*, pp. 289–291, Apr. 1999.
- Á. I. Csurgay and W. Porod, "Network representation of coupled molecular arrays," in *Proc. Eur. Conf. Circuit Theory Design, ECCTD'99*, Stresa, 1999.
- A. J. Stone, *The Theory of Intermolecular Forces*, Oxford, U.K.: Clarendon, 1997.

- [24] G. H. Bernstein, G. Bazán, M. Chen, C. S. Lent, J. L. Merz, A. O. Orlov, W. Porod, G. L. Sneider, and P. D. Tougaw, "Practical issues in the realization of quantum-dot cellular automata," *Superlatt. Microstructures*, vol. 20, pp. 447–459, 1996.
- [25] W. Cen, P. Lindenfeld, and T. P. Fehlner, "On the interface of metal-metal multiple bond compounds and organometallic clusters," *J. Amer. Chem. Soc.*, vol. 114, pp. 5451–5452, 1992.



Árpád I. Csurgay (M'87–SM'90–F'93) received the Dipl.Eng. and Ph.D. degrees in electrical engineering from the Technical University of Budapest, Hungary, in 1959 and 1964, and the D.Sc. degree from the Hungarian Academy of Sciences in 1973, respectively.

He is a Professor at the Department of Electromagnetic Theory, Technical University of Budapest, and since 1996, he has been a part-time Visiting Professor at the Electrical Engineering Department, University of Notre Dame, affiliated with the Nano Devices Group. From 1959 to 1980, he was with the Research Institute for Telecommunication, Budapest, engaged in research on microwave and later on microelectronic devices and circuits, and also served as director of research. In 1966–1967, he was with the Electrophysics Department of the Polytechnic Institute of Brooklyn as a postdoctoral fellow. From 1980 to 1985, he was with the Computer and Automation Institute of the Hungarian Academy of Sciences, and from 1985 to 1993, he served as an elected Secretary at the Academy. Since 1963, he has been teaching courses at the Technical University of Budapest as a part time lecturer in electromagnetics and physical electronics. His research interests include electromagnetic device modeling, nanoelectronic device and circuit simulation, and physical realizability of signal processors.

Dr. Csurgay has been one of the Deputy Editors of the International Journal of Circuit Theory and Its Applications, since 1973. He is a Member of the Hungarian Academy of Sciences, Member of Academia Europaea (European Academy of Sciences, London), Member of the Academia Scientiarum et Artium Europaea, Salzburg, and Fellow of IEEE. He has received the Eötvös Award, the Pázmány Award, and the Széchenyi Award. He has been the Chairman of the Circuits, Systems and Computers Chapter of the Hungary Section of the IEEE.



Wolfgang Porod (M'86–SM'90) has received the M.S. and Ph.D. degrees from the Universität Graz, Austria, in 1979 and 1981, respectively.

He is a Professor at the Department of Electrical Engineering, University of Notre Dame. From 1979 to 1981, he was affiliated with the Institut für Theoretische Physik, Universität Graz, from 1981 to 1983, he was with the Department of Electrical Engineering, Colorado State University, and from 1983 to 1986, with the Department of Electrical Engineering, Arizona State University. His research interests include solid state physics and its applications to solid state electronics, quantum devices and architectures for nanoelectronics, and limits imposed by the laws of physics on computation. He is one of the founders of the NanoDevices Group and the Center for Nanoscience and Technology at the University of Notre Dame.

Dr. Porod has received the Promotio sub auspiciis Praesidentis Austriae Award, and the Alexander von Humboldt Fellowship Award. He is a Senior Member of IEEE, and also Member of the American Institute of Physics and the Society of the Sigma Xi.



Craig S. Lent has received the A.B. degree in physics at the University of California, Berkeley, and the Ph.D. degree in solid state physics at the University of Minnesota, Minneapolis-St. Paul, in 1978 and 1984, respectively.

He is a Professor at the Department of Electrical Engineering, University of Notre Dame. In 1986, he joined the faculty at the University of Notre Dame, Notre Dame, IN, where he is now a Professor of Electrical Engineering. His research interests include RHEED oscillations, deep level defects in semiconductors, and semiconductor quantum devices. He is one of the founders of the NanoDevices Group and the Center for Nanoscience and Technology at the University of Notre Dame.