

## Signal processing by pulse-driven molecular arrays

Árpád I. Csurgay<sup>\*,†,‡</sup>, Wolfgang Porod and Balázs Rakos

*Center for NanoScience and Technology, Electrical Engineering Department, University of Notre Dame,  
275 Fitzpatrick Hall, Notre Dame, IN 46556, U.S.A.*

### SUMMARY

In this paper cellular array processors composed of weakly Coulomb coupled molecules are studied. Equivalent circuits for molecules performing optically induced electron and proton transfer are presented, and pulse-driven computing architectures are proposed. The polymer-like molecular array is processing signals if it is subjected to a sequence of electromagnetic pulses of well-defined frequency, envelope and length. Programming is accomplished by selecting proper sequence of pulses. Universality of the proposed architecture for computing is demonstrated. Copyright © 2003 John Wiley & Sons, Ltd.

KEY WORDS: nanotechnology; nanoelectronics; molecular dynamics; modelling; circuit simulation

### 1. INTRODUCTION

A large number of metal-contacted nanodevices were demonstrated, however, no viable technology for large-scale integration has been suggested so far. Coulomb coupling of devices has been proposed as an alternative approach for nanodevice integration has been proposed [1].

The strongest intermolecular forces in a molecular array (e.g. forces between molecules in a polymer) are Coulomb forces.

In a recent paper [2] we introduced equivalent circuits for arrays composed of Coulomb coupled molecules. The internal electronic dynamics of the molecules have been described by quantum Markovian master equations, describing the dynamics of the devices as irreversible evolution of an open quantum system coupled to reservoirs. The state of the nuclei was

---

\* Correspondence to: Árpád I. Csurgay, Center for NanoScience and Technology, Electrical Engineering Department, University of Notre Dame, 275 Fitzpatrick Hall, Notre Dame, IN 46556, U.S.A.

‡ On leave from the Budapest University of Technology and Economics and Pázmány Péter Catholic University, Budapest, Hungary.

† E-mail: acsurgay@nd.edu

Contract/grant sponsor: US Office of Naval Research (MURI program);

Contract/grant sponsor: W.M. Keck Foundation;

Contract/grant sponsor: Hungarian National Research Fund.

characterized by classical state variables such as position and momentum. The introduction of equivalent circuits has been based on mixed quantum-classical dynamics. Equivalent circuit models for coupled arrays subject to close-to-resonance external electromagnetic fields have also been introduced in reference.

In this paper we continue the exploration of these equivalent circuits. We focus on the mixed quantum-classical dynamics of molecular arrays. We still assume that the molecules are far enough apart from each other that the overlap between their quantum-wave functions can be ignored, thus coherence is restricted to the internal dynamics. However, additional to the internal dynamics and electron transfer, studied earlier, we explore nuclear vibrations and proton switching as well. We study coupled ‘nanomechanic’ and ‘nanoelectronic’ dynamics of Coulomb coupled molecules as potential devices and circuits performing signal processing.

We envisage an array of Coulomb-coupled molecules subject to a sequence of electromagnetic pulses of well-defined frequency, shape of envelope and length. The idea that this array, in principle, can do computing is not new. Körner and Mahler [3] suggested to inducing parallel logic in arrays of quantum dots through the selective driving of resonances. Lloyd proposed a ‘Gedanken experiment’ with a ‘potentially realizable quantum computer’ by subjecting an array of weakly coupled quantum systems to a sequence of pulses [4,5]. We also studied optically pumped computing architectures, and we also proposed a physically realizable architecture [6]. However, none of the former studies looked at the impact of the nuclear vibrations and switching on signal processing.

In this paper, based on the equivalent circuit models introduced in Reference [2], we propose cellular molecular arrays as architectures for signal processing. In the arrays fast electronic switching is combined with nuclear vibrations and switching. We assume that the molecules in the arrays can be considered to be two-quantum state systems with mechanical vibration in one variable.

According to our simulations, nuclear dynamics can play a profound and helpful role in signal processing. Polymer-like arrays composed of molecules, which can be modelled as quantum-classical systems having two-electronic states and a one-dimensional nuclear vibration are promising candidates for cellular signal processing.

## 2. EQUIVALENT CIRCUIT OF A TWO-QUANTUM-STATE MOLECULE WITH ONE-DIMENSIONAL VIBRATION

In this paper we assume that the molecules in the array can be considered to be two-quantum state systems with one degree of freedom of vibration. We also assume that the potential energy surfaces of the quantum states are given, as well as the parameters of the damping channels are known. We note that the generalization for more than two quantum states and for more than one mechanical degree of freedom is straightforward.

In case of a two-state molecule,  $|\Phi_1\rangle$ ,  $|\Phi_2\rangle$ , with one mechanical degree of freedom  $R$ , the Hamiltonian matrix  $\mathbf{H}$  of a molecule depends on  $R$  as

$$\mathbf{H} = \begin{bmatrix} H_{11} & H_{12} \\ H_{12}^* & H_{22} \end{bmatrix} = \begin{bmatrix} E_1(R) & G(R) \\ G(R) & E_2(R) \end{bmatrix} \quad (1)$$

The mixed quantum-classical dynamics of each molecule can be described by a three-dimensional quantum-coherence-vector,  $\vec{\lambda}(t) = [\lambda_1(t), \lambda_2(t), \lambda_3(t)]$ , representing the  $2 \times 2$  density

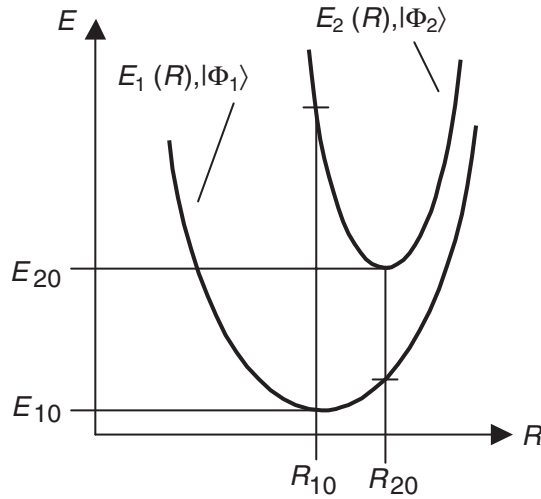


Figure 1. Potential energy surface (PES) of a two-quantum state molecule with one-dimensional mechanical vibration.

matrix of the two quantum states, and by the position of the vibrating nuclei,  $R(t)$ , together with their momentum  $P(t)$ . The Bloch equation describes the dynamics of the coherence vector

$$\hbar \frac{d\vec{\lambda}(t)}{dt} = \mathbf{\Omega} \cdot \vec{\lambda}(t) \quad (2)$$

where  $\hbar$  is the Planck constant, and  $\mathbf{\Omega}$  is the Bloch matrix

$$\mathbf{\Omega} = \begin{bmatrix} 0 & -H_{22} + H_{11} & -j(H_{12}^* - H_{12}) \\ H_{22} - H_{11} & 0 & -H_{12} - H_{12}^* \\ j(H_{12}^* - H_{12}) & H_{12} + H_{12}^* & 0 \end{bmatrix} \quad (3)$$

If the nuclear vibration has only one degree of freedom, the mechanics can be characterized by two classical dynamic equations

$$\begin{aligned} \frac{d}{dt} R(t) &= \frac{1}{M} P(t) \\ \frac{d}{dt} P(t) &= \langle \Psi | - \frac{\partial}{\partial R} (\mathbf{V}_{nn} + \mathbf{V}_{en}) | \Psi \rangle \end{aligned} \quad (4)$$

where  $R$  and  $P$  are the position and momentum of the vibration,  $M$  is the vibrating mass, and  $\mathbf{V}_{nn}$ ,  $\mathbf{V}_{en}$  are the nucleus–nucleus and electron–nucleus potential energies, respectively. They are determined by the potential energy surfaces (PES). Figure 1 shows an example of the PES of a molecule with electronic states  $|\Phi_1\rangle$  and  $|\Phi_2\rangle$ . In state  $|\Phi_1\rangle$  the energy  $E_1(R)$  is a function of the distance between the nuclei, and it is minimum at  $R=R_{10}$ . In electronic state  $|\Phi_2\rangle$  the potential energy is minimum at  $R=R_{20}$ . Note that in the excited electronic state, i.e. in state  $|\Phi_2\rangle$ , the nuclear vibration first relaxes to  $R_{20} > R_{10}$ .

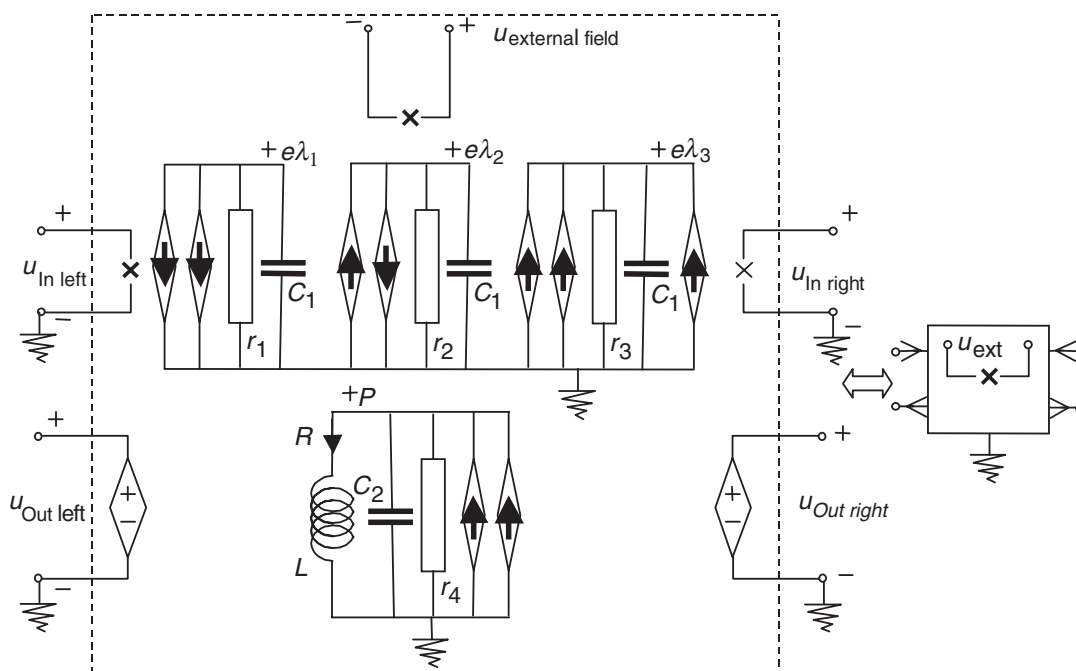


Figure 2. Equivalent circuit of a two-quantum state molecule with one-dimensional mechanical vibration.

Figure 2 illustrates the equivalent circuit model of a molecule with two quantum states and with one mechanical degree of freedom. The dynamics of the quantum state is characterized by the time-varying charges of the  $C_1$  capacitors, charges  $e\lambda_1(t), e\lambda_2(t), e\lambda_3(t)$ . The mechanical vibration follows the dynamics of the  $L-C$  resonant circuit, in which the capacitor voltage is  $P(t)$ , and the inductor current is  $R(t)$ . The quantum and classical dynamics are coupled to each other, and also to the Coulomb field of the neighbours.

The molecular array is pumped by an external electromagnetic field. In the equivalent circuit it is represented by a generator,  $u_{\text{external field}}(t)$ .

We assume that the Coulomb field of a molecule's neighbours perturbs  $(H_{22} - H_{11})$ , and the perturbation depends not only on the distances but on the quantum states of the neighbours as well. The external electromagnetic field interacts with the dipole moment of the molecule according to Rabi's semi-classical theory, and adds a time-varying term to  $(H_{12} - H_{12}^*)$ .

The perturbation terms and the field-to-molecule interaction depend on the specifics of the molecules and on their location and orientations in the array, but in this paper we assume that the parameters of the circuit model had been determined before we started the simulation of networks. The internal electronic dynamics of the molecules, according to the quantum Markovian master equations, is an irreversible evolution of an open quantum system coupled to a heat bath.

$$\hbar \frac{d\vec{\lambda}(t)}{dt} = \mathbf{\Omega}\vec{\lambda}(t) + \mathbf{R}\vec{\lambda}(t) + \vec{k}$$

$$\begin{aligned}\frac{d}{dt}R(t) &= \frac{1}{M}P(t) \\ \frac{d}{dt}P(t) &= \langle \Psi | -\frac{\partial}{\partial R}(\mathbf{V}_{\text{nn}} + \mathbf{V}_{\text{en}}) | \Psi \rangle - \alpha \cdot P\end{aligned}\quad (5)$$

where  $\mathbf{R}$  and  $\vec{k}$  are the damping matrix and damping vector, respectively, and  $\alpha$  characterizes the mechanical relaxation. The value of  $\alpha$  is zero or positive, the damping matrix and vector have been studied and determined for various damping channels. Their general forms are

$$\mathbf{R} = \begin{pmatrix} -\gamma_1 & \alpha & \beta \\ \alpha & -\gamma_2 & \delta \\ \beta & \delta & -\gamma_3 \end{pmatrix}, \quad \mathbf{k} = \begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix}\quad (6)$$

with the constraint that the matrix  $\mathbf{A}$  composed of the elements of  $\mathbf{R}$  and  $\mathbf{k}$

$$\mathbf{A} = \begin{pmatrix} \frac{1}{2}(\gamma_1 + \gamma_2 - \gamma_3) & \alpha + jk_3 & \beta + jk_2 \\ \alpha - jk_3 & \frac{1}{2}(\gamma_1 - \gamma_2 + \gamma_3) & \delta + jk_1 \\ \beta - jk_2 & \delta - jk_1 & \frac{1}{2}(-\gamma_1 + \gamma_2 + \gamma_3) \end{pmatrix}\quad (7)$$

should be positive semidefinite. This imposes a set of inequalities that the damping parameters should satisfy.

The simplest model of dissipation relies on three constants of relaxation, on the temperature  $T$ , on the electronic ( $\tau$ ), and on the nuclear relaxation ( $\alpha$ ). Parameters  $\tau$  and  $\alpha$  depend on the specific environment of the molecular array. In the equivalent circuit the dissipation caused by the environment is represented with resistors  $r_1$ ,  $r_2$  and  $r_3$ . In Figure 2 all couplings are modelled by proper controlled sources.

The state equations with the simplest model of dissipation describing the dynamics of the equivalent circuit read as

$$\begin{aligned}\hbar \frac{d\vec{\lambda}(t)}{dt} &= \mathbf{\Omega} \vec{\lambda}(t) - \frac{\hbar}{\tau} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix} + \frac{\hbar}{\tau} \begin{bmatrix} 0 \\ 0 \\ 2 \tanh \frac{\Delta E}{k_B T} \end{bmatrix} \\ \frac{d}{dt}R(t) &= \frac{1}{M}P(t) \\ \frac{d}{dt}P(t) &= \langle \Psi | -\frac{\partial}{\partial R}(\mathbf{V}_{\text{nn}} + \mathbf{V}_{\text{en}}) | \Psi \rangle - \alpha P(t)\end{aligned}\quad (8)$$

### 3. DRIVING COULOMB-COUPLED MOLECULES BY PULSES

A two-state quantum system oscillates between its two eigenstates if it is excited by a close to resonance electromagnetic pulse of different duration (Rabi oscillation). If the frequency  $\omega = (E_2 - E_1)/\hbar$  and the duration of the pulse in the Rabi scale is  $\pi$  (Pi-pulse), the system switches into its other eigenstate. The presence of vibration and dissipation does not correspond anymore to the ideal Rabi case, nevertheless, pulses can be constructed to control the switching of molecules [7]. The frequency of the pulse should remain close to resonance, the shape of its envelope, and its duration should be designed. Simulations based on our equivalent circuit show that the model well approximates the phenomena called Rabi oscillation

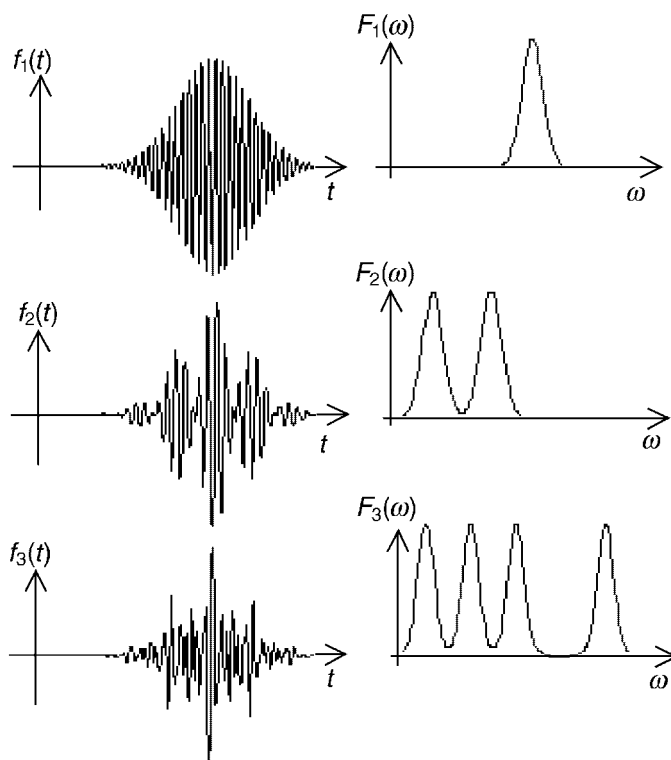


Figure 3. Chirps and their frequency spectra.

even in case of vibration and mechanical switching. Figure 3 shows the types of switching chirps together with their Fourier spectra. Chirp  $f_1(t)$  is an amplitude-modulated monochromatic field; chirp  $f_2(t)$  is the superposition of two, chirp  $f_3(t)$  of four chirps of different frequencies.

If a molecule is in its ground state and the nuclear vibration is negligible, i.e.  $R \cong R_{10}$ , then a pulse of frequency close-to-resonance  $\omega_1 = [E_2(R_{10}) - E_{10}]/\hbar$  will switch the molecule into its excited state. However, in the excited state the nuclei will be far from  $R_{20}$ , thus a vibration will start, which relaxes to  $R \cong R_{20}$ . Note that during this relaxation the energy difference between the two states has changed significantly, i.e.  $\omega_2 = [E_{20} - E_1(R_{20})]/\hbar \neq \omega_1$ , thus a pulse with frequency  $\omega_1$  does not switch the molecule back to its ground state. We need to change the frequency to  $\omega_2$  in order to switch the molecule back.

Figure 4 illustrates the selectivity of a  $H_2$  molecule, as a switch. We applied an  $\omega_2$ -chirp at  $t = 500$  fs. The molecule did not switch. On the other hand, a  $\omega_1$ -chirp at  $t = 1000$  fs did switch the molecule from state 1 to 2. The  $\omega_1$  chirp at  $t = 1500$  fs did not, but the  $\omega_2$ -chirp applied at  $t = 2000$  fs did switch the molecule back to state 1.

The Coulomb fields of the neighbouring molecules perturb the energy differences between the ground and excited states, thus it changes the frequency needed to switch the molecule. The Coulomb field depends not only on the distances but on the state of the neighbours as

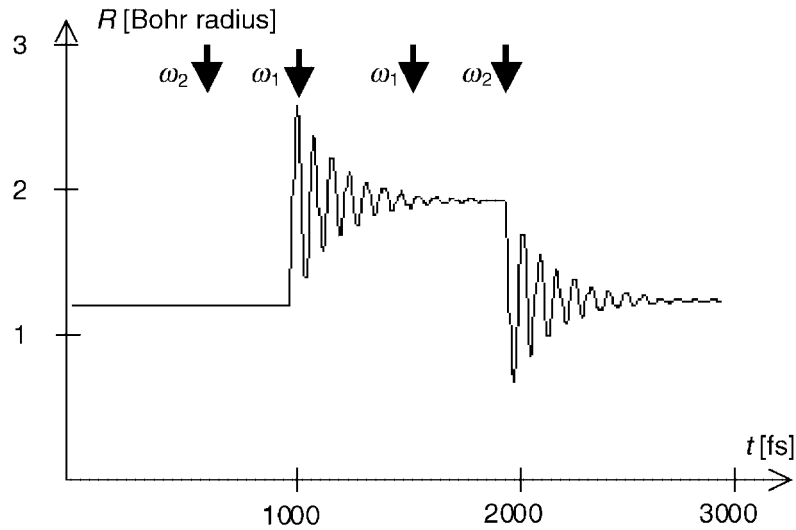


Figure 4. Hydrogen molecule flashed with chirps of frequency  $\omega_1$  at  $t_0 = 1000$  and  $1500$  fs, and with chirps  $\omega_2$  at  $t_0 = 500$  and  $2000$  fs. Selectivity is observed.

well. We have studied the effects on switching of the frequency, shape of the envelope, and the length of the pulse. Simulations indicate that in polymer-like molecular chains switching of a molecule can be induced selectively depending on the state of its neighbours. Different frequencies are needed to switch a molecule if: (i) both neighbours are in ground states, (ii) one neighbour is in excited state, one is in ground state and (iii) both neighbours are in their excited states.

Our simulations suggest that pulse-driven ('chirp-controlled') quantum-classical dynamics of molecular arrays can be approximated with our circuit model, and this model can be used to study potential architectures for signal processing.

If we introduce a combined chirp [introduced on Figure 3 as  $f_2(t)$ ] such that both frequencies,  $\omega_1 = [E_2(R_{10}) - E_{10}]/\hbar$  and  $\omega_2 = [E_{20} - E_1(R_{20})]/\hbar$  are present in the chirp, then the same combined chirp switches the molecule from state 1 to 2 and back from state 2 to 1. Figure 5 illustrates this 'invertible' switching. First, we excite the state with a chirp  $(\omega_1, \omega_2)$ , then the same  $(\omega_1, \omega_2)$  chirp imposed later switches the state back.

#### 4. SIGNAL PROCESSING WITH ONE-DIMENSIONAL ARRAYS OF PULSE-DRIVEN MOLECULES

First, we envisage a one-dimensional molecular array (chain) composed of two-state molecules. The transition between states involves both quantum and mechanic transitions:

$$\text{State 1: } |\Phi_1\rangle, R_{10} \Leftrightarrow \text{State 2: } |\Phi_2\rangle, R_{20} \quad (9)$$

In a chain of molecules the switching frequencies at the end of the chain are different from those at the internal sites of the chain, because at the end there is only one neighbour.

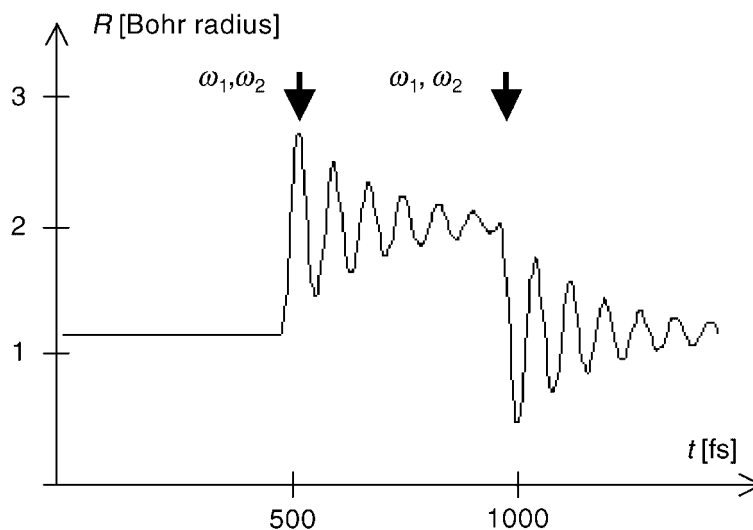


Figure 5. Switching of a molecule with a combined chirp ( $\omega_1, \omega_2$ ).

Molecules at the boundary have four chirp frequencies depending on the state of their neighbours and on their own state. A molecule at an internal site of the chain has two neighbours, thus it has six chirp frequencies depending on its own state and on the Coulomb effect of its neighbours. Let us refer to the state of the neighbours by an upper and to the state of the molecule itself by a lower index. The four chirp frequencies of the molecule at the boundary are  $\omega_1^0$ ,  $\omega_1^1$ ,  $\omega_2^0$ , and  $\omega_2^1$ . The six chirp frequencies of a molecule at an internal site of the chain are  $\omega_1^{00}$ ,  $\omega_2^{00}$ ,  $\omega_1^{01} = \omega_1^{10}$ ,  $\omega_2^{01} = \omega_2^{10}$ ,  $\omega_1^{11}$  and  $\omega_2^{11}$ .

The molecular chain is programmed by a sequence of chirps of specific frequencies. We assume that at the beginning of processing the chain is in its ground state  $(0, 0, 0, \dots)$ . First, the initial data are loaded by a sequence of chirps. The algorithm of the signal processing is performed by the next sequence of chirps. A simple example is the loading of a bit onto the second molecule of a chain. The loading is performed by a sequence of chirps with frequencies  $\omega_1^0$ ,  $\omega_1^{01}$  and  $\omega_2^1$ . Note that this sequence transforms the initial ground state as  $(0, 0, 0, \dots) \rightarrow (1, 0, 0, \dots) \rightarrow (1, 1, 0, \dots) \rightarrow (0, 1, 0, \dots)$ .

Figure 6 shows the distance between the nuclei of the first ( $R_1$ ) and the second ( $R_2$ ) molecule of a long chain when a  $\omega_1^0$ -chirp is flashed at  $t=0$ ,  $\omega_1^{01}$ -chirp at  $t=500$  fs, and  $\omega_2^1$ -chirp at  $t=1000$  fs. Indeed, after the sequence of three pulses,  $\omega_1^0$ ,  $\omega_1^{01}$  and  $\omega_2^1$ , the state of the chain is  $(0, 1, 0, \dots)$ .

It has been shown [4] that a universal ‘replacement’ computer can be implemented as an ideal chain formed from three different types of molecules  $ABCABCABC\dots$ , if selective and invertible addressing of  $A$ ,  $B$  and  $C$  are insured. The combined chirp mentioned above facilitates the inversion of a logic-state with the same chirp. Using our circuit model, we have shown that by a proper sequence of chirps any given binary string can be loaded onto the chain  $ABCABCABC\dots$ , composed of molecules with two quantum states and one mechanical state. Simulations suggest that a universal replacement computer can be realized as a pulse-driven polymer-like molecular array.

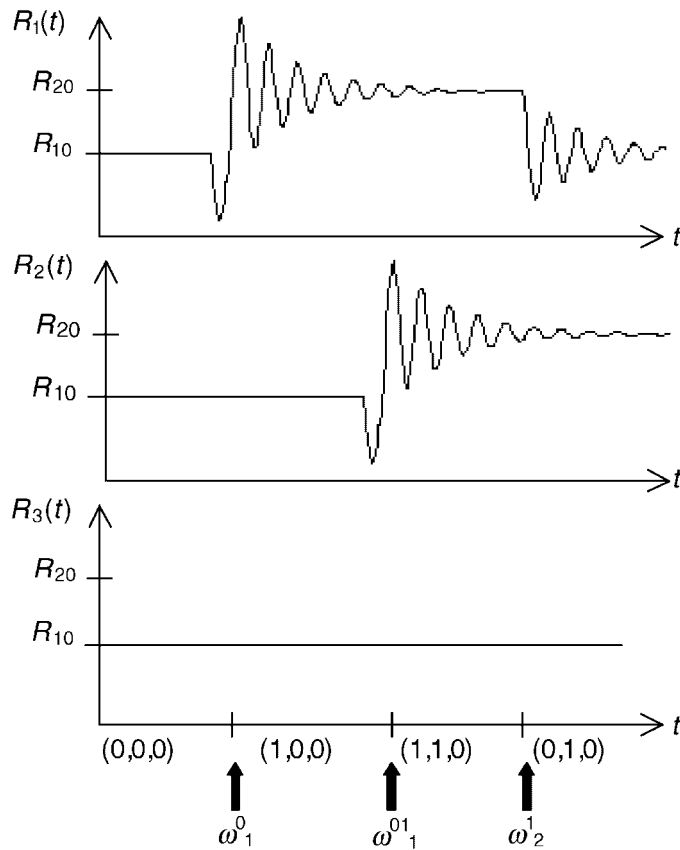


Figure 6. Loading a bit on the second molecule of a one-dimensional molecular chain by chirps  $\omega_1^0$ ,  $\omega_1^{01}$  and  $\omega_2^1$ .

We relied on the theorem that any invertible logic function can be realized with the successive application of a logic unit, called Fredkin-gate [10]. A Fredkin-gate is a binary gate with three inputs,  $X$ ,  $Y$ ,  $Z$  and three outputs,  $X'$ ,  $Y'$ ,  $Z'$  in which  $X'$  always is equal to  $X$ , and  $Y' = Y$ ,  $Z' = Z$  if  $X = 0$ ;  $Y' = Z$ ,  $Z' = Y$  if  $X = 1$ . That is, if  $X = 0$ , all three inputs go through unchanged; if  $X = 1$ , the second and third input are exchanged. A Fredkin-gate causes an exchange of bits between two units conditioned on the value of a third. Fredkin-gates suffice to give the logical operations AND, OR, NOT and FANOUT.

Our simulations verified that a series of combined chirps,  $\omega_C^{10}$ ,  $\omega_C^{11}$ ,  $\omega_B^{11}$ ,  $\omega_C^{10}$  and  $\omega_C^{11}$  induces the operation of a Fredkin gate on the molecular triple  $ABC$ .

## 5. TWO-DIMENSIONAL ARRAYS OF PULSE-DRIVEN MOLECULES

Figure 7 illustrates the structure of a pulse-driven majority gate. The program of the majority gate function is composed of four consecutive chirps:  $\omega_1^{10}$ ,  $\omega_1^{1100}$ ,  $\omega_1^{1110}$ ,  $\omega_1^{10}$ . For inputs  $(0, 0, 0)$

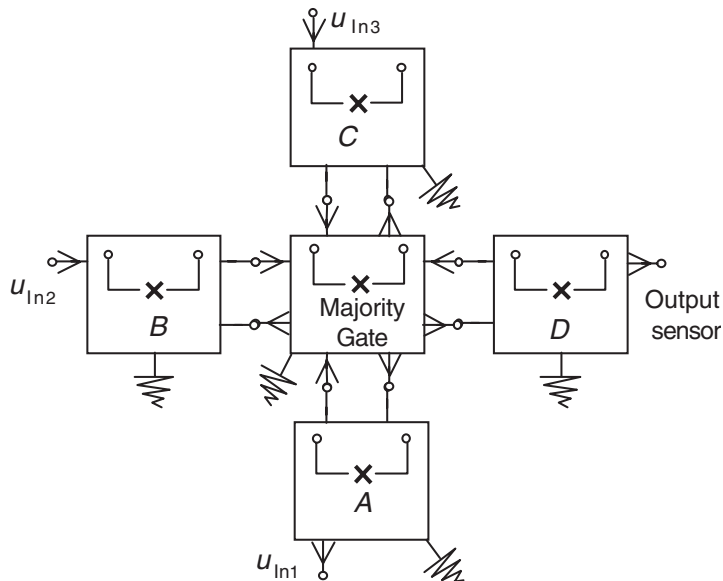


Figure 7. Majority gate composed of five molecules, programmed with a series of chirps  $\omega_1^{10}$ ,  $\omega_1^{1100}$ ,  $\omega_1^{1110}$  and  $\omega_1^{10}$ .

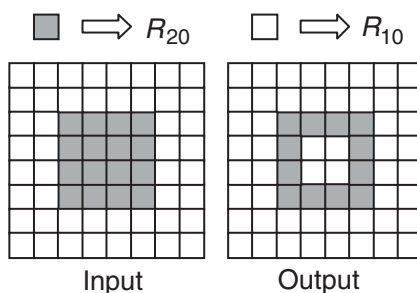


Figure 8. Input and output of a molecular array flashed by a chirp of frequency  $\omega_0^{1111}$ .

and  $(1,0,0)$ , the output molecule stays in its state 0. However, for inputs  $(1,1,0)$  and  $(1,1,1)$  it is switched from 0 to 1.

Figure 8 shows a two-dimensional array with a square-shape-like initial pattern on it. Note that the switching frequencies of the molecules inside the square significantly differ from the frequencies of the molecules at the edge of the shape and at outside. A properly designed chirp can selectively switch the molecules inside. The edge of the input pattern emerges as the output.

The dynamics in molecular chains and arrays is not just binary. Fast switching between quantum eigenstates is combined with slow mechanical vibration and switching. In the pulse-driven arrays non-linear waves are propagating and interfering, patterns are emerging. It

has been suggested that two-dimensional cellular arrays have unique computing potential [11,12].

However, the signal processing potential of polymer-like pulse-driven molecular arrays has not been explored as yet. Simulations, based on the circuit model introduced in our paper, suggest that the non-linear waves propagating and interfering in the molecular arrays resemble the spatial-temporal dynamics proposed and demonstrated as cellular non-linear networks [13,14].

## 6. CONCLUSIONS AND OUTLOOK

In this paper simulations of interacting quantum and mechanical dynamics of Coulomb coupled molecules subject to external electromagnetic pulses are presented. The state of the nuclei has been characterized by classical state variables such as position and momentum, and the internal quantum dynamics of the molecules by quantum Markovian master equations of finite-state systems. Coherence has been restricted to the internal dynamics of the molecules, which can result in internal quantum state and also in mechanical, e.g. in proton switches.

Equivalent circuits for pulse-driven molecules were presented, and the quantum-classical dynamics of the arrays have been approximated as the dynamics of coupled non-linear analog circuits. Fast electronic switching, combined with slow mechanical nuclear vibrations, induced by pulses (chirps) have been analysed, and strong selectivity with respect to switching on/off, and also with respect to the state of the neighbours has been observed.

A ‘Gedanken experiment’ has been performed with a chain of polymer-like molecules. Simulations verified the potential realizability of a replacement computer. In two-dimensional molecular-arrays-rich dynamics resembling spatial-temporal flows in cellular non-linear networks have been found.

## ACKNOWLEDGEMENTS

This work was supported in part by grants from the U.S. Office of Naval Research (MURI program), the W. M. Keck Foundation, and also by the Hungarian National Research Fund (OTKA).

## REFERENCES

1. Porod W, Lent CS, Bernstein GH, Amlani I, Snider GI, Merz JL. Quantum-dot cellular automata computing with coupled quantum dots. *International Journal of Electronics* 1999; **86**(5):549–590.
2. Csurgay ÁI, Porod W. Equivalent circuit representation of arrays composed of Coulomb-coupled nanoscale devices. *International Journal of Circuit Theory and Applications* 2001; **29**:3–35.
3. Körner H, Mahler G. Optically driven quantum networks: applications in molecular electronics. *Physical Review B* 1993; **48**(4):2335–2346.
4. Lloyd S. A potentially realizable quantum computer. *Science* 1993; **261**:1569–1571.
5. Lloyd S. Programming pulse driven quantum computers. 17 December 1999, arXiv:quant-ph/9912086.
6. Csaba Gy, Csurgay ÁI, Porod W. Computing architecture composed of next-neighbour-coupled optically pumped nanodevices. *International Journal of Circuit Theory and Applications* 2001; **29**:73–91.
7. Gordon J, Rice SA. Active control of the dynamics of atoms and molecules. *Annual Review of Physical Chemistry* 1997; **48**:601–641.
8. Meyer R, Ernst RR. Transitions induced in a double minimum system by interaction with a quantum mechanical heat bath. *Journal of Chemical Physics* 1990; **93**(8):5518–5532.
9. Meyer R, Ernst RR. Hydrogen transfer in double minimum potential: kinetic properties from quantum dynamics. *Journal of Chemical Physics* 1987; **86**(2):784–801.

10. Feynman RP. *Feynman Lectures on Computation*. Addison Wesley: Reading, MA, 1996.
11. Zuse K. *Rechnender Raum, Schriften zur Datenverarbeitung*, vol. 1. Freidr. Vieweg & Sohn: Braunschweig, 1969.
12. Chua LO. *CNN: A Paradigm for Complexity*. World Scientific: Singapore, 1998.
13. Chua LO, Roska T. *Cellular Neural Networks and Visual Computing*. Cambridge University Press: Cambridge, 2002.
14. Roska T. Computational and computer complexity of analogic cellular wave computers. *Proceedings of the IEEE-CNNA-2002*, Frankfurt, July, 2002.