Active Nanoelectronic Devices and Circuits

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1 Introduction

Three ways of nanodevice interconnection have been suggested so far. Metal-contacted devices in the meso-scale range (10 to 100 nanometer), such as nano-transistors, resonant tunneling devices, RTDs and metal-dot single electron transistors, SETs, can be interconnected with wires. As long as each device has metal contacts, i.e. they are all embedded into 'heat baths', conventional interconnection with wires is possible. In this case circuit dynamics following the conservation laws of charge and energy obeys Kirchhoff's laws. However, nanodevices not metal contacted, e.g. quantum-dot arrays and artificial atoms and molecules can be coupled by inter-device electron transport or by electromagnetic fields. In case of wiring and inter-device electron transport the current flow generates unavoidable dissipation. An alternative approach of device integration is electromagnetic field interaction between the devices, such as coupling by Coulomb- or by magnetic forces. This approach can bring devices closer to each other and significantly decrease dissipation.

Field-coupled nanoelectronic discrete devices and simple circuits, such as wires, switches and logic gates, based on quantum phenomena have been demonstrated. However, there has been no viable design procedures for large-scale integration proposed.

If both field-coupled and metal-contacted nanodevices are applied in the same circuit, the physical interface between a field-coupled and a metal-contacted nanodevice can be represented as a classical electromagnetic circuit. The boundary conditions on the side of the metal contacted device are defined by the metal contacts, on the side of the field-coupled device by the electric or magnetic field of generated by the nanodevices.

In reference [1] we concluded that integrated circuits composed of field-coupled and metal-contacted nanodevices do have equivalent circuit representations, thus circuit theory techniques can be applied to build device models, to simulate and to aid the design of large-scale nanoelectronic integrated circuits.

Circuit models of nanodevices having electronic and mechanic (nuclear or phonic) degrees of freedom were presented. An approximate model of individual isolated devices (molecules), models for structures with weak coupling between nanodevice neighbors; models of the thermal bath and damping channels, and models for the external forces were presented (Figure 1).

2 Nanodevices with two electronic states and one vibrational degree of freedom

It has been shown [1], [2], [3], that the electronic or magnetic state at time t of any 2-level open quantum system can be described by a state-vector $\vec{\lambda}(t)$, called 'coherence vector', representing the Hermitean (2x2) density matrix $\boldsymbol{\rho}(t)$. The time-evolution from an initial state $\boldsymbol{\rho}(0)$ is described by a completely positive semigroup preserving hermiticity, trace and positivity of $\boldsymbol{\rho}(t)$ for $0 \le t < \infty$. For quantum Markovian dynamics the general mathematical form of the state equation for a nanodevice with two

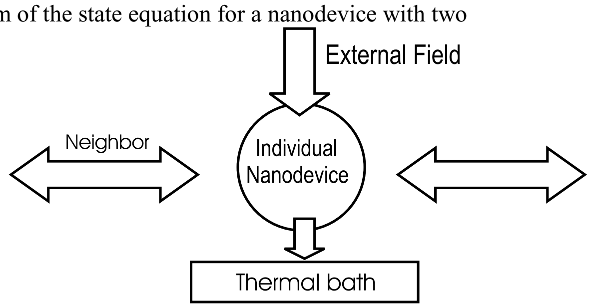

Figure 1.

electronic eigen-states and one vibrational (phonon-like) degree of freedom has been given as

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

$$\frac{\mathrm{d}}{\mathrm{d}t}R(t) = \frac{1}{M}P(t), \tag{1}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}P(t) = -\frac{1}{2}(1-\lambda_3)\frac{\partial E_1(R)}{\partial R} - \frac{1}{2}(1+\lambda_3)\frac{\partial E_2(R)}{\partial R} - \alpha \cdot P,$$

where $\boldsymbol{\Omega}$ is the Bloch matrix of the corresponding conservative system, $\mathbf{R}$ and $\vec{k}$ are the damping matrix and damping vector, respectively , and α characterizes the nuclear relaxation. The value of α is zero or positive, the damping matrix and vector have been studied and determined for various damping channels. Their general forms are

$$\mathbf{R} = \begin{pmatrix} -\gamma_1 & \alpha & \beta \\ \alpha & -\gamma_2 & \delta \\ \beta & \delta & -\gamma_3 \end{pmatrix}, \qquad \mathbf{k} = \begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix}, \tag{2}$$

with the constraint that the matrix **A** composed of the elements of **R** and **k**

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$$\mathbf{A}=\begin{pmatrix} \frac{1}{2}(\gamma_1+\gamma_2-\gamma_3) & \alpha+\mathrm{j}k_3 & \beta+\mathrm{j}k_2 \\ \alpha-\mathrm{j}k_3 & \frac{1}{2}(\gamma_1-\gamma_2+\gamma_3) & \delta+\mathrm{j}k_1 \\ \beta-\mathrm{j}k_2 & \delta-\mathrm{j}k_1 & \frac{1}{2}(-\gamma_1+\gamma_2+\gamma_3) \end{pmatrix} \quad (3)$$

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

This set of mixed quantum-classical equations describes the time-evolution of the state of a nanodevice. The coherence vector determines the electronic evolution in the depth of the density matrix, thus the expectation values of measurements are determined by it. The phonon (or nuclear) vibration and relaxation are coupled to the electronic dynamics through λ_3. Notice that the nanodevie's state equations resemble circuit dynamics. Equation (1) could be the state equation of a nonlinear circuit with state variables $\lambda_1, \lambda_2, \lambda_3, R$ and P. In Figure 2 we presented the equivalent circuit of a two electronic-state and one vibrational degree-of-freedom nanodevice. The couplings between the electronic and vibrational states are illustrated by the λ_3 and R -dependence of the circuit parameters.

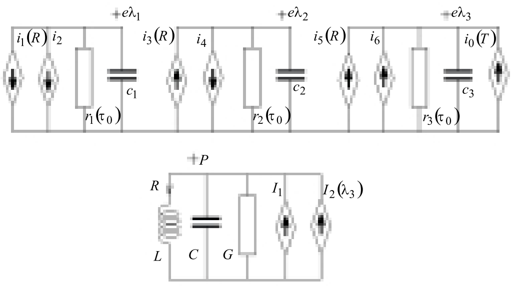

Figure 2

The equivalent circuit represents a mixed quantum-classical dynamics. A very fast electronic sub-circuit shown on the upper part of the figure is coupled to a slow nuclear vibration through the current I_2, which is generated by the voltage $\frac{e}{C}\lambda_3$. A feedback from the nuclear dynamics is expressed in the *R*-dependence of the controlled-source currents.

2. Modeling of field-coupled nanodevices

The experimental frame in which we run (or test) a nanocircuit in case of a field-coupled array of nanodevices (or molecules) assumes a macroscopic embedding, an input and an output. These could be for example two microelectronic circuits which set the input and measure the output of a field-coupled array. The macroscopic embedding has to be designed to set the input boundary conditions as a field, and to sense the output field generated by the array. We assume that both the input and output macroscopic systems are interfaced to the array through metal contacted devices. At the input the voltages on metal contacts generate the electric field, and at the output the electric field of the nanodevices generate voltages on the metal contacts.

The physical interfaces between field-coupled devices and input-output units are modeled as equivalent circuits as well. The boundary conditions at the metal contacted devices are defined by the geometry of the metal contacts driven by voltages of the embedding circuits. The field generated by the metal contacts interacts with the dipoles and quadrupoles of the field-coupled devices. The interaction is assumed to be classical, thus classical electromagnetic techniques can be used to develop the circuit model of the interface.

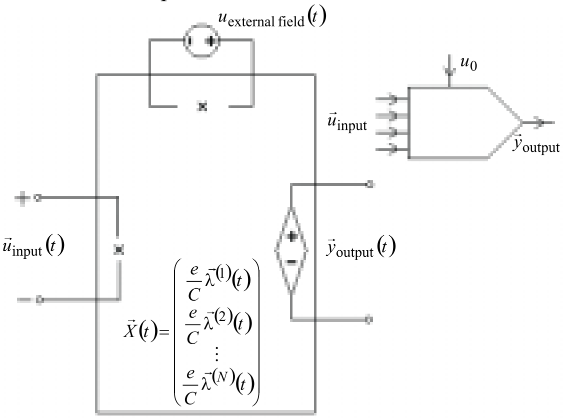

Figure 3

Figure 3 illustrates the model of the input and output of an array. In general the input is a time-varying electric field generated by a metal contacted input circuit. Looking back from the array, it can always be represented by a vector of λ_3'-s of the nanodevices ($I_1, I_2, \ldots$ denote the input ports)

$$\vec{u}_{\text{input}} = \left(\frac{e}{C}\lambda_3^{(I_1)}, \frac{e}{C}\lambda_3^{(I_2)}, \ldots \right). \quad (4)$$

The external field will be represented by an independent time-varying voltage source $\vec{u}_{\text{external field}}(t)$. The measured output is also a vector of the λ_3'-s ($O_1, O_2, \ldots$ denote the output ports)

$$\vec{y}_{\text{output}} = \left(\frac{e}{C}\lambda_3^{(O_1)}, \frac{e}{C}\lambda_3^{(O_2)}, \ldots \right). \quad (5)$$

Note that *e/C*, i.e. the electron's charge divided by a capacitance has voltage dimension thus the inputs and outputs are virtual voltages indeed. The internal electronic state variables are composed of the coherence vectors and the nuclear coordinates. If the nuclear vibration can be neglected and the number of molecules in an array is N_{mol}, then the number of state variables, i.e. the dimension of vector $\vec{\lambda}(t)$ is $3N_{mol}$. A device's model in an array depends on the properties of the individual molecules and on the geometry of the two-dimensional cluster in which the molecules are located.

First, we envisage an empty cellular array, with specified raster geometry, and specified local coordinate systems at each cell. The distances between the origins of the local coordinate systems are given together with local orientations. We also specify the individual isolated molecules with their models located in their local coordinate system. The number of output-ports of a molecule depends on the number of stationary eigenstates, and it is equal to the number of its polarization-voltages. In case of a two-state molecule this number is 1, for a three-state molecule it is 2, etc. Next, we assign to each nanodevice as many input ports as the sum of the output ports of its neighbors. The cellular array defines the maximum number of neighbors a molecule can have. If every neighboring cell is filled in by a nanodevice then all input ports are excited. However, if a neighboring cell is empty, there will be zero polarization-voltage at the corresponding input port. This way we can define a model for a nanodevice in such a way, that the model is invariant on the neighbors, i.e. the model itself does not depend on whether a neighboring cell is filled by a device or it is empty. If the geometry of the cluster, together with the local coordinate systems including the device orientations is fixed, a hierarchy of equivalent circuit models can be built.

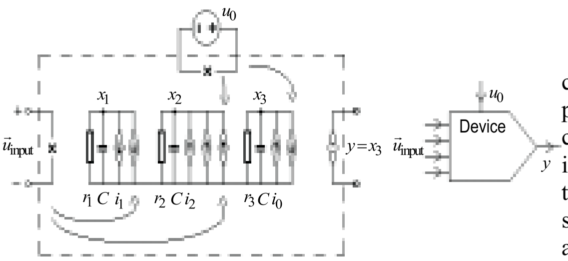

Figure 4

We shall illustrate the procedure leading to a hierarchy of models. We start with a simple example shown in Figure 4. A two-electronic-state nanodevice is located in a two-dimensional cluster. We assume that no vibrations take place. The number of output ports is one, the maximum number of neighbors is 8, thus the dimension of the input voltage-vector is 8.

Figure 5 shows the equivalent circuit of a field-coupled line composed of nanodevices such as presented on Figure 4. In case of a line a device in the midst of the line has only two neighbors, thus the input vector is two-dimensional. However, the first device of a line can have more than one neighbor on its left, and the last one can have more than one neighbor on its right. To have an equivalent circuit model of a line we have to leave open the number of input-ports at the first and at the last nanodevice of the line, because we do not know them. In our example we assumed that no more that four cells are filled at the input and at the output of the line.

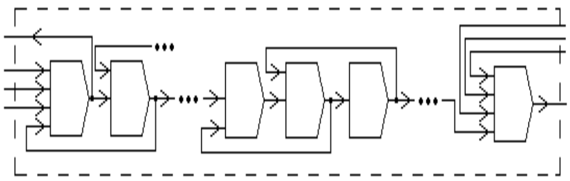

Figure 5

Figure 6 shows the equivalent circuit of a majority gate composed of four two-state nanodevices. The signals flow in the direction of the thicker line, and there is a feedback to the neighbors shown by the thinner lines.

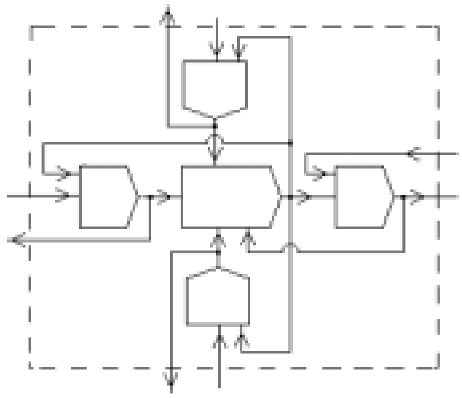

Figure 6

A computing architecture composed of Coulomb-coupled optically pumped two-state nanodevices has been proposed [5]. A new four-level device, built from two coupled two-state devices called 'nanodevice-pair,' is introduced. Simulations on the equivalent circuit models of two-dimensional arrays composed of nanodevice-pairs suggest that non-reciprocal pipelining wires, ring oscillators and NAND gates can be built. It has been shown that the optically pumped nanodevice-pairs do not stack in meta-stable states, and they restore logic levels.

Figure 7 shows the double-device. We have demonstrated that it is possible to design a selective optical excitation in such a way that a series of consecutive flashes irradiated on the whole array, will push the input logic state to the output resulting in the required functionality. Examples have been given illustrating the possibility of designing a class of 'pipelined' logic. 'Wires' composed of nanodevice-pairs, 'ring oscillator' type arrangements, and a NAND gate, as examples have been demonstrated.

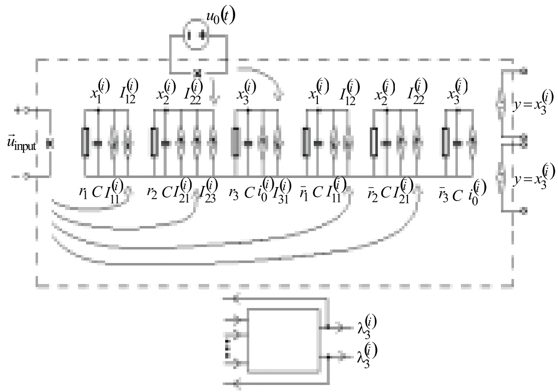

Figure 7.

3. Interfaces between Coulomb-coupled and metal contacted nanodevices

We have seen that in a nanoelectronic integrated circuit the input electromagnetic field of a field-coupled molecular array is set by a metal contacted microelectronic circuit, and the output electric field is measured similarly by voltages on metal contacts. The time-varying electromagnetic field $\vec{E}(\vec{r},t)$ generated by the metal contacted input circuit couples to the dipoles and quadrupoles of the nearest nanodevices in the array. This relation is represented as an equivalent circuit of the interface. To find this circuit we have to solve a classical electromagnetic problem. In the first approximation the problem is quasi-static, and the equivalent circuit can be composed of ideal transformers. In general, the equivalent circuit is a linear, reciprocal reactance circuit representing the coupling between the electric field generated by the metal contacted microelectronic circuit and the state-varaible of the nanodevice.

At the output the field generated by the nanodevice is sensed and measured by the metal contacts of the output microelectronic circuit. The coupling of the field to the voltages of the metal-contacted devices can be represented as a linear, reciprocal reactance circuit, similarly to the input. Figure 8 illustrates the equivalent circuits of both interfaces, both of them acting as linear filters.

However, the measurement at the output ports introduces an additional, non-local, damping channel, because the macroscopic system with its huge number of particles enforce similar effects on the nanodevice array as that of the thermal bath.

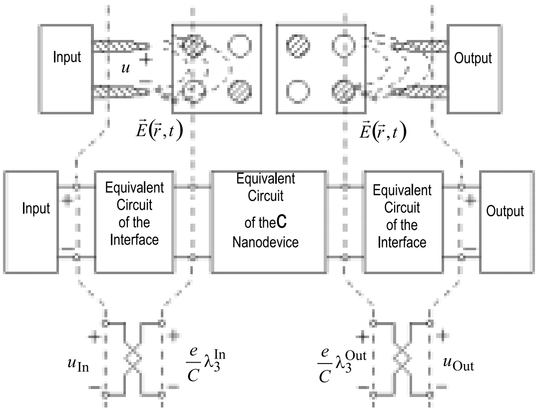

Figure 8

Acknowledgment

This work was supported in part by the Office of Naval Research MURI Program, and a grant from the W. M. Keck Foundation.

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