

TOWARD NANOELECTRONIC SYSTEMS INTEGRATION

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ABSTRACT

A novel nanometer-scale electronic technology, called nanoelectronics is emerging. Nanoelectronic discrete devices, such as resonant tunneling diodes and transistors, single-electron transistors, bistable quantum-cells, quantum interference devices, etc. have been proposed and built. Technology and physics of the devices are reasonably well understood, but there exists a gap between device physics and nanoelectronic systems integration. In this paper it will be shown that in case of local quantum coherence, i.e. if coherence is restricted to the internal dynamics of Coulomb-coupled devices, system dynamics can be described by a set of coupled ordinary nonlinear differential equations. In this case virtual charges, voltages and currents, obeying Kirchoff's equations, can be assigned to the dynamic variables of the state equations, thus circuit models can be introduced. We also show that edge-driven arrays performing ground state computing are locally passive systems if the Coulomb-coupled devices are excited by the input signals only. In order to perform signal processing or computing, external energy should be pumped into the array, and the pumped array should be locally active. Adiabatic pumping is one way of injecting energy to the signal path.

1. INTRODUCTION

In nanoelectronics, systems integration is a challenge. Nanoelectronic discrete devices are with us, nevertheless, there has been – for the time being – no viable large-scale systems integration proposed and demonstrated with minimum feature size in the ten nanometer range, and speed over terahertz.

To build a processor on a chip, a large number of discrete devices should be coupled. If each device has metal contacts, i.e. they are all embedded into heat baths, then conventional interconnection with wires is possible, and standard form of Kirchoff's laws prevail. But in most cases the unavoidable electromagnetic fields generated by the wires destroy quantum device performance. Proposals that overcome this difficulty, published so far, prefer next-neighbor-Coulomb coupling instead of wiring [1,2].

Promising system architectures exploiting the so called 'edge-driven ground state relaxation' have been proposed, and device and systems models based on Hubbard-type Hamiltonians and the Hartree-Fock approximation have been presented [3, 4, 5]. Simulation of simple functional units, such as an inverter or a majority gate can be based on these models, but they are not applicable in case of larger integrated systems.

In this paper, it will be shown that in case of local quantum coherence, i.e. if coherence is restricted to the internal dynamics of the Coulomb-coupled devices, system dynamics is described by a set coupled ordinary nonlinear differential equations. In this case virtual charges, voltages and currents, obeying Kirchoff's equations, can be assigned to the dynamic variables of the state equations. Circuit models can be introduced; thus the circuit paradigm can serve as a bridge between device physics and integrated system design. The interfaces between Coulomb-coupled and metal contacted devices can be modeled in a similar way.

Local activity of devices is a necessary condition of signal processing [6]. We shall show that edge-driven arrays performing ground state computing are locally passive systems if the Coulomb-coupled devices are excited by the input signals only. In order to perform signal processing or computing, external energy should be pumped into the array in addition to the signal input, and the pumped array should be locally active for the perturbation of small-signal inputs. Adiabatic pumping is one way of injecting energy to the signal path.

2. INTEGRATED SYSTEMS COMPOSED OF WEAKLY COULOMB-COUPLED ARTIFICIAL (OR NATURAL) MOLECULES

Nanoelectronics 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

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needs new approaches, and (3) as device size shrinks the increasing power dissipation becomes intolerable.

According to a proposal of the nanodevices group of the University of Notre Dame (1) quantum phenomena could be used for nanoscale signal processing; (2) next-neighbor-coupled cellular networks are promising as architectures for nanoelectronic processors, and (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 [3, 4, 5].

We envisage a molecular array composed of molecules described by a finite set of basis states. The molecules are far enough apart from each other that the overlap between their wave functions can be ignored. Relatively weak intermolecular forces govern the interactions between molecules; it is natural to describe their effects using perturbation theory.

The perturbation consists of the electrostatic interaction between the molecules (electrons and nuclei). Indeed, all of the contributions to the interaction energy between molecules, except for the negligible magnetic terms, derive ultimately from the Coulomb interactions between their particles. Coulomb interactions between charges localized inside spheres around the charges can be specified by the interactions between multipoles representing the charge-distributions inside the isolated spheres.

3. DYNAMICS OF MOLECULES

Let us select a molecule from the array. The Liouville–von Neumann equation, describes its electronic dynamics

$$\frac{\partial \rho}{\partial t} = \mathbf{H}\rho - \rho\mathbf{H} \quad (1)$$

where ρ is the density operator of the molecule, and \mathbf{H} is the Hamilton operator, depending on the properties of the molecule itself and also on the effects of the neighboring molecules. The operators in Eq.1 are represented by matrices of complex valued elements.

The density matrix depends on time, and its time dependence can be represented by s real-valued time-functions $\lambda_1(t)$, $\lambda_2(t)$, ... $\lambda_s(t)$. The algebra of the n -dimensional unitary groups $SU(n)$ gives a technique to determine them. These functions can be considered as components of a s -dimensional vector, $\vec{\lambda}$, called coherence vector. If the Hamilton operator is Hermitian, it can also be represented by an s -dimensional vector \vec{H} , and the trace of \mathbf{H} .

In case of two-state molecules, the dimension of the state vector is $s=3$, $\vec{\lambda} = (\lambda_1, \lambda_2, \lambda_3)$, $\mathbf{H} = (H_1, H_2, H_3)$, $\text{Tr}\{\mathbf{H}\} = H_0$,

$$\rho = \frac{1}{2} \begin{bmatrix} 1 - \lambda_3 & \lambda_1 - j\lambda_2 \\ \lambda_1 + j\lambda_2 & 1 + \lambda_3 \end{bmatrix} \quad (2)$$

$$\mathbf{H} = \frac{1}{2} \begin{bmatrix} H_0 - H_3 & H_1 - jH_2 \\ H_1 + jH_2 & H_0 + H_3 \end{bmatrix}$$

As long as the dynamics of the molecule is lossless, Eq.1 can be transformed into the Bloch equation

$$\hbar \frac{\partial \vec{\lambda}(t)}{\partial t} = \vec{H} \times \vec{\lambda}. \quad (3)$$

The expectation value of the energy content of a molecule can be expressed as

$$E = \text{Tr} \rho \mathbf{H} = \frac{1}{n} \text{Tr} \mathbf{H} + \frac{1}{2} \vec{H} \vec{\lambda}. \quad (4)$$

Dynamical equation (Eq.3) assumes that there is no coupling to the environment other than interactions between the molecules. The coupling between the coherence vector $\vec{\lambda}$ of one molecule and its neighbors occurs through the Hamiltonian vector \vec{H} .

Interactions with the environment randomize the quantum mechanical phase and cause inelastic (dissipative) relaxation. These effects can be built into the model through the generalized Bloch equations,

$$\frac{d \vec{\lambda}^{(k)}}{dt} = \vec{\Gamma}^{(k)} \times \vec{\lambda}^{(k)} - \frac{1}{\tau_{in}} \left(\frac{1}{\tanh \Delta^{(k)}} \vec{\lambda}^{(k)} + \frac{\vec{\Gamma}^{(k)}}{|\vec{\Gamma}^{(k)}|} \right), \quad (5)$$

where we have introduced a temperature ratio $\Delta^{(k)} = \frac{E_0^{(k)}}{k_B T}$ and a relaxation time τ_{in} ; k_B is the Boltzmann constant and T is the temperature [7, 8].

4. MULTIPOLE REPRESENTATION OF MOLECULAR INTERACTIONS

Let us consider at a selected single molecule (k) of the array and assume that its unperturbed states are known. First, let us study the perturbation of molecule (k) by another molecule (l) in its neighborhood. The perturbed Hamiltonian then is $H^{(k)} = H_0^{(k)} + H'^{(k)}$, where the operator $H'^{(k)}$ describes the Coulomb effect of molecule (l) on molecule (k). By introducing the vector $\vec{R} = \vec{R}^{(l)} - \vec{R}^{(k)}$ and the gradients of $\frac{1}{R}$, where $R = |\vec{R}|$,

$$T = \frac{1}{R}, \quad T_{x_i} = \nabla_{x_i} \frac{1}{R}, \quad T_{x_i x_j} = \nabla_{x_i} \nabla_{x_j} \frac{1}{R},$$

$$T_{x_i x_j x_m} = \nabla_{x_i} \nabla_{x_j} \nabla_{x_m} \frac{1}{R},$$

$$T_{x_i x_j x_m x_n} = \nabla_{x_i} \nabla_{x_j} \nabla_{x_m} \nabla_{x_n} \frac{1}{R},$$

we can express the interaction operator in terms of the multipoles of molecules (k) and (l) [9]

$$H'^{(kl)} = \frac{1}{4\pi\epsilon_0} \left(\sum_{i=1}^3 p_{x_i}^{(k)} p_{x_i}^{(l)} + \frac{1}{3} \sum_{i=1}^3 \sum_{j=1}^3 Q_{x_i x_j}^{(k)} q_{x_i x_j}^{(l)} + \dots \right)$$

where

$$p_{x_i}^{(l)} = \sum_{j=1}^3 T_{x_i x_j} p_{x_j}^{(l)} + \frac{1}{3} \sum_{m=1}^3 \sum_{n=1}^3 T_{x_i x_m x_n} Q_{x_m x_n}^{(l)} + \dots,$$

$$q_{x_i x_j}^{(l)} = \sum_{m=1}^3 T_{x_i x_j x_m} p_{x_m}^{(l)} + \frac{1}{3} \sum_{m=1}^3 \sum_{n=1}^3 T_{x_i x_j x_m x_n} Q_{x_m x_n}^{(l)} + \dots,$$

and $\vec{p}^{(k)}$ and $\mathbf{Q}^{(k)}$ are the dipole and quadrupole moments of molecule (k), and $\vec{p}^{(l)}$ and $\mathbf{Q}^{(l)}$ those of molecule (l).

The interaction terms have been derived for pairs of molecules. However, they are based on the Coulomb interactions between nuclear and electronic charges, which are strictly additive, so the formulae can be generalized to an assembly of molecules by summing over the neighbors.

5. NONLINEAR CIRCUIT ANALOGY OF WEAKLY COUPLED MOLECULES

In a weakly coupled molecular array the dynamics of each molecule can be described by the dynamic equation, which in $\vec{\lambda}$ is a first order nonlinear ordinary differential equation. The instantaneous power entering a molecule is

$$p(t) = \frac{dE}{dt} = \frac{d}{dt} \left(\frac{1}{2} \vec{H} \cdot \vec{\lambda} \right).$$

We can build up an analogy between circuit models and molecules by formally assigning a 'charge' vector $\vec{q} \triangleq e\vec{\lambda}$ to each molecule, and viewing $(1/e)\vec{H}$ as the formal 'voltage' vector $\vec{v} = (1/e)\vec{H}$. Note that both $\vec{\lambda}$ and \vec{H} are real valued vectors of dimension $s = n^2 - 1$, thus we can assign to a molecule with n eigenstates s charges as time-varying real state variables.

Establishing an analogy between weakly-coupled arrays and circuits has advantages. First, large-scale arrays can be simulated by standard circuit-simulators. Second, functions of known and useful circuit arrays could be studied from the point of view of molecular realizations, and realizability of useful functions with weakly coupled molecular arrays could be explored.

6. SIGNAL DRIVEN MOLECULAR ARRAYS ARE LOCALLY PASSIVE

An edge-driven molecular array has been investigated near equilibrium ground state by small signal excitation. The linear small signal model of the V-I relation is a frequency dependent admittance means that the system is locally passive. In the simplest case the 1-port admittance is

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

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

This admittance is positive real (PR). (It is the admittance of two RLC passive circuit.) The criteria of positive reality are clearly met. From the positive reality it follows that time-invariant two-state molecules are locally passive, thus the arrays composed of them cannot possess multiple equilibria or cannot realize signal-power-gain.

7. LOCAL ACTIVITY OF MOLECULAR ARRAYS

We have seen that Coulomb-coupled molecules may be viewed as strongly nonlinear devices. The strength of the coupling, i.e. the off-diagonal element γ of the Hamiltonian matrix, 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 sufficiently high γ , the polarization can be fixed near zero.

This control can be used for adiabatic pumping, thus realizing time-varying systems. It can be shown that adiabatic pumping can inject energy into the signal path, thus it converts the molecular array into a locally active system, which enables us to build systems with signal power gain and multiple equilibria [7]. Other mechanisms to convert molecular arrays into locally active regime have been and are being investigated.

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