Information coding and intramolecular integration of logic functionality

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ABSTRACT

We investigate the feasibility of integrating Boolean logic within molecules. Physical characteristics of nano-scale electronics like high contact resistances and the huge potential for further miniaturization are the main arguments for advocating this approach. Here, we analyze the possibility of directly implementing the constraints separating the decision regions equivalent to a Boolean function through controlling the coefficients of the transmission matrix – that is, through molecular design. A first analysis of the possible ways of mapping information processing on molecules leads us to a negative result. Special techniques for linearization are possible with an exponential cost. This result has considerable implications as it requires implicitly including decoherence in the design of molecular devices..

Keywords: molecular electronics, architecture, information coding.

1 INTRODUCTION

Although molecular electronics has great potential, the feasibility of this technology will be conditioned by the possibility of building complex circuits. In this context, intramolecular integration of logic functionality has been advocated for a plethora of reasons, ranging from the huge miniaturization potential to avoiding problems related to high contact resistances [1]. On the technological versant rapid progress has been made during the last years in manipulating either carbon nanotubes or organic molecules but we still lack a formal framework for information processing at nanoscale. As fabricating and measuring simple devices is gradually mastered, this gap is now resented as a major bottleneck for working towards the scalability of various proposals.

All state of the art proposals for nanoscale architectures either present global architectural solutions [2],[3],[4] or simply try to translate classical concepts like resistor-diode logic at nanoscale. But as the electronic phase coherence length is larger then the size of the nanoscale devices there are changes in some fundamental architectural aspects like their composition; modifications of the conductance superposition law have been shown in [5]. Thus, studying the passage from macroscopic diode logic AND gate to the monomolecular counterpart, Stadler and al. [6] have obtained four logical levels instead of two. For instance, for the passage from a macroscopic PGLA half-adder to its molecular counterpart, it was found that the variation of the output current due to the input signal is about 40 times smaller than that due to the position of the connecting wires.

In this paper we point out a critical problem for the intra-molecular integration of complex functionality: the linearity of the transmission matrix formalism.

In Section II of the paper we point out how the linearity constraint is set by the physical model. Section III discusses the negative implications of this constraint on the possibility of mapping logic on molecules and proposes a solution using Support Vector Machines. Conclusions are discussed in Section V.

2 FORMAL FRAMEWORK

We have argued earlier that, in order to fully take advantage of architectural paradigms, one should follow the monomolecular approach rather than the hybrid one.

A generic methodology for mapping a logic function on molecules is illustrated in Figure 1. Thus, we adopt the transmission matrix as an intermediate representation between the logical functionality of a molecule and it's a*b initio* description.

While due to its generality the NEGF formalism is now being chosen by many authors for modeling molecular transport, we restrict our representation to the Landauer-Büttiker formalism due to its being more illustrative for the following argumentation.

In a system having N pads the currents flowing, for instance, in terminal p is

$$i_p = \frac{2e}{h}\sum_{q=1}^{N}\overline{T}_{pq}\cdot\left(f_p - f_q\right), \quad p = \overline{1,N} \tag{1}$$

explicitly it is a system of N equations with N variables

$$\begin{cases} i_1 = \dfrac{2e}{h}\sum\limits_{q=1}^{N}\overline{T}_{1q}\cdot\left(f_1 - f_q\right) \\ i_2 = \dfrac{2e}{h}\sum\limits_{q=1}^{N}\overline{T}_{2q}\cdot\left(f_2 - f_q\right) \\ \vdots \\ i_N = \dfrac{2e}{h}\sum\limits_{q=1}^{N}\overline{T}_{Nq}\cdot\left(f_N - f_q\right) \end{cases} \tag{2}$$

where $\overline{T}_{pq}$ is the transfer function from terminal q to terminal p at energy E, and f_p is the Fermi function for terminal p:

$$f_p(E,\mu_p) = \frac{1}{\exp\left(\frac{E-\mu_p}{k_B T}\right)+1} \tag{3}$$

The electro-chemical potential is given by the product of the electron charge and the potential on the terminal p;

$$\mu_p = eV_p \tag{4}$$

If we were to work in a single-energy mode then the effective current through terminal p would be equal to i_p. Otherwise the current will result after integrating over the entire energy range

$$I_p = \int i_p(E)\cdot dE \tag{5}$$

2.1 Information coding

The functionality of a circuit consists of its ability to modify currents and voltages through what is called input-output characteristic. In "classical" microelectronics this is usually a voltage (current) transfer function (V-V, I-I), a transimpedance (I-V) or a transadmittance (V-I). The first collapse of this type of "coding" was reported in microwave circuit theory. At very high frequencies the information carriers are not V or I but rather the incident and reflected power waves, namely a or b. More interesting is the scattering matrix formalism that was successfully used in describing the behavior of microwave multi-terminal circuits.

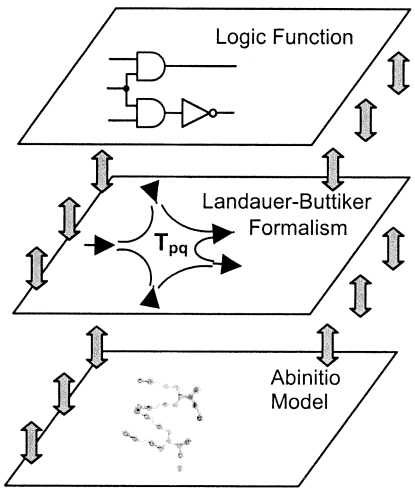

Figure 1: A framework for intra-molecular logic

In molecular electronics, we are tempted to do the same thing. We might see the padded molecule as a multiport device [1] and then try to use a formalism that will properly describe the transfer between two arbitrary terminals. We could even establish the potential (V) and current (I) as information carriers. But the most important point is that the resulting formalism should be consistent with quantum effects specific to molecular electronics. Fortunately for us virtually the same problem was tackled by the advent of mesoscopic physics, as a theory for modeling charge transport in presence of quantum effects.

In the following we ignore the inability of Landauer-Büttiker formalism to model non-equilibrium transport and consider for the moment just a single-energy mode. In this case by setting all N currents at each terminal all N functions $f_1,\ldots, f_N$ are uniquely determined by the system (2), which is linear in f_i. Moreover, because f_p is bijective with respect to μ_p and also to V_p, it results in the latter also being uniquely determined. If we consider the output to be for instance V_p, because f_p is a linear combination of all currents, it follows that

$$V_p = \frac{k_B T}{e}\ln\left(\exp\left(\frac{E}{k_B T}\right)\cdot\frac{\sum_q a_q I_q}{1-\sum_q a_q I_q}\right) \tag{6}$$

In the followings we will argue that this is the only nonlinear type of function that we can realize based on the assumptions we have made earlier: coherent transport and single-energy mode.

2.2 The linearity constraint

From the equations in system (2) one can obtain in the left side term any combination of currents and Fermi functions which satisfy only two constraints: they must be N and have distinct indexes. The right side term of the resulting system will contain the complements. I_p and f_q are said to be complementary if $q=p$. Consequently, the system (2) can be rewritten using a hybrid matrix H. For instance:

$$\begin{cases} I_1 = h_{11}f_1 + h_{12}I_2 + \ldots + h_{1N}f_N \\ f_2 = h_{21}f_1 + h_{22}I_2 + \ldots + h_{2N}f_N \\ \vdots \\ I_N = h_{N1}f_1 + h_{N2}I_2 + \ldots + h_{NN}f_N \end{cases} \tag{7}$$

Setting N_1 different currents and N_2 different potentials on the terminals of the system (with $N_1+N_2=N$) will determine the left side term of system (7). By choosing as output a current Ip (let it be I_2) we have a totally linear dependence of the fixed currents and Fermi functions.

$$I_2 = a_1 I_1 + a_2 f_2 + \ldots + a_N I_N \tag{8}$$

If we consider though a potential output (i.e. V_1) then we have

$$f_1 = a_1 I_1 + a_2 f_2 + \ldots + a_N I_N \tag{9}$$

which implies

$$V_1 = \frac{k_B T}{e} \ln\left[\exp\left(\frac{E}{k_B T} \right) \cdot \frac{a_1 I_1 + a_2 f_2 + \ldots + a_N I_N}{1 - (a_1 I_1 + a_2 f_2 + \ldots + a_N I_N)} \right] \tag{10}$$

Before we get to see the approximation power of the two functions, (8) and (10), we should have some considerations on coefficients a_i. They form the line p of the inverse matrix H^{-1} if the output is considered being either the current or the potential at terminal p. Each element of H matrix is usually a rational function in transfer functions $\overline{T}_{pq}$. By the inversion process the elements of H^{-1} will contain all N^2–N transfer functions, that is

$$h_{ij}^{-1} = g_{ij}(\overline{T_{12}}, \ldots, \overline{T_{1N}}, \ldots, \overline{T_{N1}}, \ldots, \overline{T_{N,N-1}}) \tag{11}$$

where we had to ignore $\overline{T}_{pp}$ terms, and g_{ij} is a determined function. Thus, in the optimal case, each coefficient will depend on all N^2-N transfer functions, giving us the same number of freedom degrees to play with.

2.3 Boolean functions

In this section we will focus on the functional approximation power of either (8) or (10). The inputs are as previously stated N_1 currents and N_2 potentials and the output is one current or potential from the complementary set.

Note that, since we leave a total freedom in choosing the inputs and the output, we are intrinsically exploring the **coding space** in an exhaustive manner. Simply stated we fully characterize the information coding potential of this physical level.

We are interested in mapping a Boolean function on the Landauer-Buttiker formalism. By expanding a Boolean function as multi-linear polynomial we have

$$f(x_1, \ldots, x_N) = \sum_i a_i^{(1)} x_i + \sum_{i \neq j} a_{ij}^{(2)} x_i x_j + \ldots + \sum_{i1 \neq \ldots \neq iN} a_{i1 \ldots iN}^{(N)} x_i \cdot \ldots \cdot x_N \tag{12}$$

Consequently, the Boolean function approximation problem is strictly conditioned by the ability to realize all weighted product terms of the equation (12). From now on we **will designate by nonlinearity, one of these products.**

In the case of **current outputting** (8), it is impossible to realize any of the nonlinearities of (12), regardless of the choice of the coefficients a_i. That is explainable by observing that each individual mixed partial derivative of any order is zero,

$$\frac{\partial^k I_p}{\partial q_1 \cdots \partial q_k} = 0, \; k \geq 2 \tag{13}$$

where q_i is a current or a potential, and at least one pair q_i, q_j doesn't represent the same variable.

On the other hand reserving an input for each product term will yield 2^N inputs!

If our output is a potential we could try to benefit from the nonlinearity introduced by the inverse Fermi function, f_p^{-1} of the equation (10). Performing a Taylor expansion on this function will result in an infinite length series. Each coefficient is a partial derivative of this function with respect to its inputs and depends only on parameters $a_1, \ldots, a_N$. In a very optimistic frame, so that we have full access in modifying these parameters individually, we still have only N of them and that is totally insufficient for satisfying all 2^N nonlinearities. We should have at least 2^N parameters to fit our Boolean function!

3 COPING WITH LINEARITY

The strongest consequence of the linearity constraint is the impossibility of implementing arbitrary Boolean functions.

3.1 Implications of linearity

Undoubtedly, the simplest approach would be trying to map Boolean logic onto this intermediate representation

$$(x_1, x_2) \xrightarrow{f} f(x_1, x_2) \tag{14}$$

$$\Updownarrow$$

$$\begin{pmatrix} \varphi \\ \varphi \\ \varphi \\ f(x_1, x_2) \end{pmatrix} = \begin{pmatrix} ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ 1 \\ 0 \end{pmatrix}$$

where $x_1, x_2 \in \{0,1\}$

Here, $f(x_1,x_2)$ is a logic function of Boolean variables x_1,x_2. Implementing f becomes equivalent to finding the coefficients of the S-matrix that allow obtaining f as a linear combination of x_1 and x_2. While very simple, this approach is limited by the impossibility of implementing a universal set of Boolean gates within a linear formalism. A classical counter-example is the XOR gate – one can easily see that the equation $aXORb = \alpha a + \beta b + \gamma$ can never be satisfied [7]. Moreover as the composition of two molecular devices will remain a linear operator it is not possible to decompose non-linear functions the classical way: $a\_xor\_b = a\bar{b} + \bar{a}b$. Thus, the consequence of linearity is

the impossibility to map directly an arbitrary Boolean function on a transmission matrix.

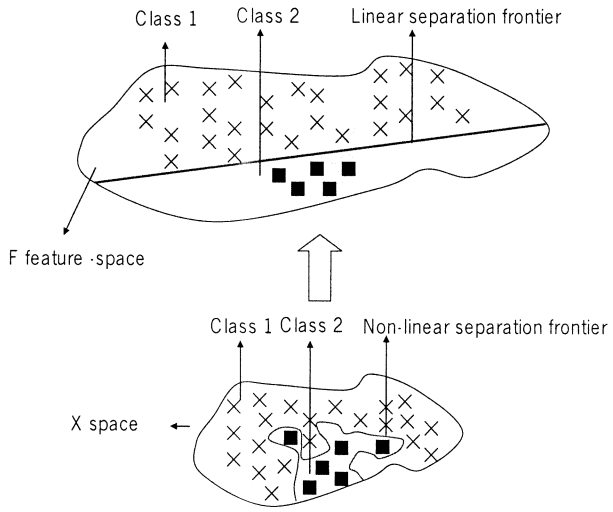

Figure 2: Achieving linear separability by passing to a feature space

3.2 Support Vector Machines

Support Vector Machines were developed as a neural networks technique to cope with non-separable data. The basic idea is illustrated in Figure 2. Given a space X where one wants to implement a non-linear classification it is possible to pass to a higher dimension space F, where the classification problem becomes linear. As sometimes the dimensionality of the feature space F increases exponentially one can translate the problem into the dual space of F. Here the dimensionality of F disappears – however it is translated into the number of constraints needed to specify the hyper-planes separating the decision regions of the classification.

3.3 Boolean function linearization

Using Support Vector Machines for Boolean classification has been extensively investigated. We give here a basic example of reducing an arbitrary Boolean classification to a linear separable problem.

Since any Boolean function can be written in Disjunctive Normal Form it can be represented as a weighted sum of all possible conjunctions

Definition 1 $\phi(x) \overset{def}{=} (\phi_1,...,\phi_l), l = 2^d - 1$ with: $\phi_i = \prod_{i_1 \neq i_2 \neq ... i_k} x_{i_1} x_{i_2} ... x_{i_k}$, such as the set of the ϕ_i vectors covers all possible combinations of all degrees *k*.

Theorem. For any Boolean function *g(x)* there is a hyperplane $f(z) = \sum_{i=1}^{2^d-1} w_i z_i$ that satisfies the following condition for any $x \in \{0,1\}^d$ $g(x) = 1 \Leftrightarrow f(\phi(x)) = 1$ and $g(x) = 0 \Leftrightarrow f(\phi(x)) = -1$

The demonstration of this theorem follows easily form the fact that the ϕ_i vectors are a basis of the hyper-space representing Boolean vectors of length *n* and thus any Boolean vector can be written as a linear combination of ϕ_i.

3.4 The cost of using SVM

As one can easily see from above, in theory the cost of transforming a Boolean function into a linear classification is **exponential**. However this is only a superior limit - in practice it depends on the maximum degree of the multi-linear polynomial representing the Boolean function.

4 CONCLUSION

We pointed out that coherent transport has an intrinsic linearity constraint that restricts the logic gates that can be mapped on molecules. Techniques to cope with this constraint exist but they introduce an exponential cost. The fundamental implication of these conclusions is that work on future molecular devices should take explicitly into account decoherence and self-consistency when designing molecular devices.

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