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Controlled Electronic Transport through Branched Molecular Conductors

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Abstract

The conductance through a branched conductor placed between two electrodes is analyzed using the Landauer transport formulation within the framework of the single electron, and the tight binding approximations. Terminal side chains are expressed as self energy terms which map the branched conductor onto an effective linear chain Hamiltonian. The effect of uniform side branches on resonant zero-bias conductance is shown to be analytically solvable and particularly simple, where subtraction or addition of a single terminal site can induce an effective discontinuity in the main linear chain or can effectively decouple the side branch from the conductor. Manipulating the "effective length" of a side branch by a local terminal gate potential, control of the small bias current through the branched conductor is demonstrated.

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I. Introduction

In the past decade single molecules were embedded in electrical circuits and the corresponding electric currents passing through such molecular junctions were measured[1-7]. Fundamental interest as well as the technological potential of molecular electronics devices led to rapid progress in this field. Electron transport through a single molecule is similar in principle to electron transport through quantum dots or wires[8], but molecular junctions are especially challenging due to the richness of geometrical structures[7] and configuration changes (electronic-nuclear coupling[9-16]). In particular, conductors with branched (non linear) molecular structures are most interesting, suggesting new possibilities for manipulating the transport and for observing new physical phenomena.

Branched conductors are associated with multiple transmission pathways and the corresponding interference effects must be accounted for in the coherent transport regime. Several quantum interference devices were proposed or fabricated in synthetic two dimensional mesoscopic systems[17] (e.g., the y-branch[18], the T-junction[19], the dual electron wave coupler[20], the two paths interferometer[21], and quantum dots arrays[22]). Quantum interference effects in electronic transport through specific pi-conjugated molecular conductors were also demonstrated theoretically[23-26].

In this work a general formulation is introduced for analyzing the effect of side branches on the transport through a branched molecular conductor. Single organic molecules[3], carbon nanotubes[2] or graphene sheets[27,28] provide natural templates for realizations of such branched molecular systems. The theoretical framework for analyzing the

transport properties is based on the Landauer formulation, invoking a tight binding model of the electronic system.

The paper is organized as follows: In section II the model of a branched conductor and the corresponding transport equations are introduced. In section III we show that the conduction through a branched conductor can be formulated in terms of an effective linear chain Hamiltonian. The approach is applied for the simple case of a uniform conductor characterized by constant on-site energies in resonance with the impact electron energy, where the mapping of the branched system onto a linear one is shown to be straight forward. In section IV we demonstrate a conductance switch based on local gating of a remote terminal site of a side branch. Conclusions are given in section V.

II. The branched conductor

Let us consider a branched molecular conductor of the type illustrated in Fig. 1a, invoking a single particle tight binding framework. Each one of N electronic sites is associated with an on-site energy and hopping integrals coupling it to its nearest neighboring sites. The conductor is coupled to two semi-infinite electrodes via two terminal sites. The electrodes are modeled as semi-infinite uniform linear chains, each characterized by a chemical potential and bandwidth, denoted below as μ_L (μ_R) and $4\gamma_L$ ($4\gamma_R$) for the left (right) electrode, respectively. The corresponding hopping integrals between the conductor and the electrodes are denoted below as ξ_L, ξ_R .

Denoting the orthonormal on-site electronic states at the conductor and the J 'th electrode as $|\chi_i^{(c)}\rangle$, and $|\varphi_i^{(J)}\rangle$, respectively, the model Hamiltonian is written as follows,

$$\hat{H} = \sum_{J=c,L,R} \hat{H}_J + \sum_{J=L,R} (\hat{H}_{cJ} + \hat{H}_{Jc}), \quad (2.1)$$

where the conductor and the electrodes Hamiltonians are defined as,

$$\hat{H}_c = \sum_{i=1}^N E_i |\chi_i^{(c)}\rangle \langle \chi_i^{(c)}| + \sum_{i,j=1}^N (\gamma_{i,j} |\chi_i^{(c)}\rangle \langle \chi_j^{(c)}| + h.c.) \quad (2.2)$$

$$\hat{H}_J = \sum_{i=1}^{\infty} \mu_J |\varphi_i^{(J)}\rangle \langle \varphi_i^{(J)}| + (\gamma_J |\varphi_i^{(J)}\rangle \langle \varphi_{i+1}^{(J)}| + h.c.) \quad ; \quad J \in R, L \quad (2.3)$$

where $\gamma_{i,j} \neq 0$ only for nearest neighboring sites. The coupling operators between the conductor and the electrodes subspaces are,

$$\begin{aligned} \hat{H}_{cL} &= \xi_L |\chi_1^{(c)}\rangle \langle \varphi_1^{(L)}| \quad ; \quad \hat{H}_{Lc} = \xi_L^* |\varphi_1^{(L)}\rangle \langle \chi_1^{(c)}| \\ \hat{H}_{cR} &= \xi_R |\chi_N^{(c)}\rangle \langle \varphi_1^{(R)}| \quad ; \quad \hat{H}_{Rc} = \xi_R^* |\varphi_1^{(R)}\rangle \langle \chi_N^{(c)}| \end{aligned} \quad (2.4)$$

where the left and right terminal sites of the conductor are associated with $i=1$ and $i=N$ respectively. Using the transport equations of Landauer, the current through the conductor from left to right reads[8],

$$I = \frac{2e}{h} \int_0^{\infty} dE [f_L^e(E) - f_R^e(E)] t(E), \quad (2.5)$$

where $f_J^e(E) = \frac{1}{1 + e^{(E - \mu_J)/k_B T}}$ is the Fermi distribution of electrons at the J'th electrode

(assuming only elastic scattering, the holes distributions are not considered explicitly[29]).

The properties of the molecular junction are captured in the transmission function,

$$t(E) = \text{tr}[\hat{\Gamma}_c^{(R)}(E) \hat{G}_c(E) \hat{\Gamma}_c^{(L)}(E) \hat{G}_c^\dagger(E)], \quad (2.6)$$

where the trace is evaluated within the conductor subspace[15]. The corresponding operators $\hat{G}_c(E)$, $\hat{\Gamma}_c^{(L)}(E)$ and $\hat{\Gamma}_c^{(R)}(E)$ are expressed in terms of self energies, defined as,

$$\hat{\Sigma}_J(E) = \lim_{\varepsilon \rightarrow 0} \hat{H}_{cJ} \left[\frac{1}{E - \hat{H}_J + i\varepsilon} \right] \hat{H}_{Jc} ; \quad J = R, L, \quad (2.7)$$

where,

$$\hat{G}_c(E) = \left[E - \hat{H}_c - \hat{\Sigma}_L(E) - \hat{\Sigma}_R(E) \right]^{-1}, \quad (2.8)$$

and

$$\hat{\Gamma}_c^{(J)}(E) = -2 \text{Im}(\hat{\Sigma}_J(E)) \quad ; \quad J = R, L. \quad (2.9)$$

For this model the self energy terms of the left and right electrodes read[15,30],

$$\begin{aligned} \hat{\Sigma}_L(E) &= |\chi_1^{(c)}\rangle \langle \chi_1^{(c)}| \frac{|\xi_L|^2}{2\gamma_L^2} \left[E - \mu_L - i\sqrt{4\gamma_L^2 - (E - \mu_L)^2} \right] ; \quad |E - \mu_L| < 2|\gamma_L| \\ \hat{\Sigma}_R(E) &= |\chi_N^{(c)}\rangle \langle \chi_N^{(c)}| \frac{|\xi_R|^2}{2\gamma_R^2} \left[E - \mu_R - i\sqrt{4\gamma_R^2 - (E - \mu_R)^2} \right] ; \quad |E - \mu_R| < 2|\gamma_R| \end{aligned} \quad (2.10)$$

III. The effective linear chain Hamiltonian

Here we show that within the present model the transport properties (transmission function) of a branched non linear conductor can be mapped exactly on the properties of an effective linear chain. Substituting Eqs.(2.8-2.10) in Eq.(2.6), one can see that the transmission function depends on a single matrix element of the conductor's Green function, i.e.,

$$\hat{G}_{1,N}^{*(c)}(E) = \hat{G}_{N,1}^{(c)}(E) = \langle \chi_N^{(c)} | \left[E - \hat{H}_c - \hat{\Sigma}_L(E) - \hat{\Sigma}_R(E) \right]^{-1} | \chi_1^{(c)} \rangle. \quad (3.1)$$

Let us divide the conductor space into two subspaces, introducing two projection operators[31],

$$\sum_{i=1}^N |\chi_i^{(c)}\rangle \langle \chi_i^{(c)}| = \hat{P}_m + \hat{P}_b \quad ; \quad \hat{P}_m = \sum_{l=1}^m |\chi_l^{(c)}\rangle \langle \chi_l^{(c)}| \quad (3.2)$$

\hat{P}_m projects to a subspace of the conductor which contains m sites ($m \leq N$). This subspace includes the two terminal sites which are coupled to the electrodes ($i_1 = 1$ and $i_m = N$) and a sequence of electronic sites linking between the terminal sites via a continuous linear chain. The operator \hat{P}_b projects to the complementary subspace of the conductor, which contains all the side branches coupled to particular sites along the linear chain. Using these two projection operators, Eq.(3.1) can be expressed in terms of a reduced effective Hamiltonian of the linear chain,

$$\hat{G}_{N,1}^{(c)}(E) = \langle \chi_N^{(c)} | [E - \hat{H}_m^{(eff)}]^{-1} | \chi_1^{(c)} \rangle \quad (3.3)$$

$$\hat{H}_m^{(eff)} = \hat{H}_m + \hat{\Sigma}_b(E) + \hat{\Sigma}_L(E) + \hat{\Sigma}_R(E), \quad (3.4)$$

where $\hat{\Sigma}_L(E)$ and $\hat{\Sigma}_R(E)$ were defined above (Eq.(2.10)). The Hamiltonian for the uncoupled linear chain reads,

$$\hat{H}_m = \hat{P}_m \hat{H}_c \hat{P}_m, \quad (3.5)$$

and the coupling to the side branches is captured by another self energy operator,

$$\hat{\Sigma}_b(E) = \lim_{\varepsilon \rightarrow 0} \hat{P}_m \hat{H}_c \hat{P}_b \left[\frac{1}{E - \hat{P}_b \hat{H}_c \hat{P}_b + i\varepsilon} \right] \hat{P}_b \hat{H}_c \hat{P}_m. \quad (3.6)$$

In general, there can be several (up to m) side branches attached to the main linear chain. For simplicity we assume that each (l 'th) side chain is coupled only to a single site of the main chain (denoted $|\chi_{i_l}^{(c)}\rangle$) and that the side branches are otherwise decoupled as, e.g., in Fig. 1a (the generalization for the more general case is straight forward). $\hat{\Sigma}_b(E)$ can therefore be conveniently split into additive contributions from the different side branches,

$$\hat{\Sigma}_b(E) = \sum_{l=1}^M \hat{\Sigma}_b^{(l)}(E)$$

$$\hat{\Sigma}_b^{(l)}(E) = \lim_{\varepsilon \rightarrow 0} \hat{P}_m \hat{H}_c \hat{P}_b^{(l)} \left[\frac{1}{E - \hat{P}_b^{(l)} \hat{H}_c \hat{P}_b^{(l)} + i\varepsilon} \right] \hat{P}_b^{(l)} \hat{H}_c \hat{P}_m \quad (3.7)$$

$\hat{P}_b^{(l)}$ is the projection to the subspace of l 'th side branch, where M is the number of side chains and $\sum_{l=1}^M \hat{P}_b^{(l)} = \hat{P}_b$. Denoting the first on-site state in the corresponding side branch as $|\chi_{j_l}^{(c)}\rangle$, the l 'th self energy term reads,

$$\hat{\Sigma}_b^{(l)}(E) = \sigma_b^{(l)} |\chi_{j_l}^{(c)}\rangle \langle \chi_{j_l}^{(c)}|$$

$$\sigma_b^{(l)}(E) = |\gamma_{i,j_l}|^2 \lim_{\varepsilon \rightarrow 0} \langle \chi_{j_l}^{(c)} | \left[\frac{1}{E - \hat{P}_b^{(l)} \hat{H}_c \hat{P}_b^{(l)} + i\varepsilon} \right] | \chi_{j_l}^{(c)} \rangle. \quad (3.8)$$

Using Eqs.(3.4,3.7,3.8) it follows that the effective Hamiltonian can be written as,

$$\hat{H}_m^{(eff)} = \hat{H}_m(E) + \hat{\Sigma}_L(E) + \hat{\Sigma}_R(E)$$

$$\hat{H}_m(E) = \sum_{l=1}^m (E_{i_l} + \sigma_b^{(l)}(E)) |\chi_{i_l}^{(c)}\rangle \langle \chi_{i_l}^{(c)}| + \sum_{l=2}^m (\gamma_{i_l, i_{l-1}} |\chi_{i_l}^{(c)}\rangle \langle \chi_{i_{l-1}}^{(c)}| + h.c.), \quad (3.9)$$

i.e. the effect of the l 'th side branch amounts to a change ($\sigma_b^{(l)}(E)$) in the on-site (local, potential) energy at the l 'th site of an effectively linear conductor.

Let us focus now on the case of a specific uniform side branch containing a single chain of n sites. By uniform we mean that all on-site energies are identical and equal to E_b (the hopping integral may vary between different sites). The localized states along the side chain are denoted $|\chi_{j_l}^{(c)}\rangle$; $j_l = 1, 2, \dots, n$, and the coupling to the main chain is via the

n 'th site and is denoted $\gamma_{n+1,n}$. The projection operator into the side chain is defined as,

$\hat{P}_{b,n}^{(l)} = \sum_{j_i=1}^n |\chi_{j_i}^{(c)}\rangle\langle\chi_{j_i}^{(c)}|$, and the (uncoupled) chain Hamiltonian is

$$\hat{P}_{b,n}^{(l)} \hat{H}_c \hat{P}_{b,n}^{(l)} = \sum_{j_i=1}^n E_b |\chi_{j_i}^{(c)}\rangle\langle\chi_{j_i}^{(c)}| + \sum_{j_i=2}^n (\gamma_{j_i, j_i-1} |\chi_{j_i}^{(c)}\rangle\langle\chi_{j_i-1}^{(c)}| + h.c.). \quad (3.10)$$

The effect of this side chain on the on-site energy at the main chain can be calculated analytically using the decimation renormalization method[32]. Here we start by expressing the energy-dependent correction to the on-site energy ($\sigma_b^{(l)}(E)$) in terms of the Green operator for the side-chain, using Eq.(3.8),

$$\sigma_b^{(l)}(E) = |\gamma_{n+1,n}|^2 \langle\chi_n^{(c)}| \frac{1}{E - \hat{P}_{b,n}^{(l)} \hat{H}_c \hat{P}_{b,n}^{(l)} + i\varepsilon} |\chi_n^{(c)}\rangle \equiv |\gamma_{n+1,n}|^2 G_{b,n}^{(l)}(E). \quad (3.11)$$

Then we define a hierarchy of projection operators,

$$\hat{P}_{b,n-1}^{(l)} = \hat{P}_{b,n}^{(l)} - |\chi_n^{(c)}\rangle\langle\chi_n^{(c)}|, \quad (3.12)$$

Which are used for constructing recursively the Green operator,

$$G_{b,n}^{(l)}(E) = \frac{1}{E - E_b - |\gamma_{n,n-1}|^2 G_{b,n-1}^{(l)}(E)}. \quad (3.13)$$

The recursion ends at the terminal site ($|\chi_1^{(c)}\rangle$) of the linear side-chain where,

$$G_{b,1}^{(l)}(E) = \lim_{\varepsilon \rightarrow 0} \frac{1}{E - E_b + i\varepsilon}. \quad (3.14)$$

Now let us focus on the case in which the impact electron energy is resonant with the on-site energy along the side chain. As $E \rightarrow E_b$, $G_{b,1}(E)$ diverges, $G_{b,2}(E)$ vanishes and so on, $G_{b,n}(E)$ alternates between infinity and zero as the recursion progresses.

Consequently, $\sigma_b^{(l)}(E)$ diverges for odd number of sites in the side chain (odd n), and

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3 vanishes for even values of n . This implies that for $E \rightarrow E_b$, a side chain with an odd
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6 number of sites is expressed as an effective local discontinuity in the effective linear
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9 conductor, (zero transmission) while a side chain with an even number of sites is
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11 effectively decoupled from the main chain under the same conditions. Notice that the
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13 alternations in the transmission due to coupling of a main conductor to a linear side-chain
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15 within the tight binding approximation were pointed out before[22,25,26]. These
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17 alternations were rightfully attributed to quantum interference between the direct and the
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19 indirect scattering pathways.
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23 Our analysis can be further applied when the side branch bifurcates. Consider a side-
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25 branch containing a main branch chain, coupled to secondary terminal side chains.
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27 Treating these terminal chains according to the above analysis, we conclude that each
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29 terminal side-chain can be effectively decoupled from the main branch chain (for an even
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31 number of sites) or it can result in an effective discontinuity in the main branch chain (for
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33 an odd number of sites). For example, consider the uniform branched conductor with
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35 geometry as presented in Fig. 1a for $E \rightarrow E_b$. Eliminating decoupled terminal side-chains
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37 or replacing them by discontinuities (according to the corresponding number of sites in
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39 each side chain) an effective linear conductor can be obtained recursively, as illustrated in
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44 Figs. 1b,1c.

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46 This analysis suggests that the effective linear conductor Hamiltonian may depend on the
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48 number of sites present in a remote side branch, and thus the conductance properties (i.e.
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50 the transmission function) may be controlled by manipulating the length of terminal side
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52 branches. For demonstration, consider a branched uniform conductor similar to the one
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54 presented in Fig. 1 above, but missing one terminal site at the first branch from the left.
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Repeating our analysis, as illustrated in Fig. 2, one obtains a discontinuity along the effective linear conductor, meaning that in this case, the transmission vanishes for $E \rightarrow E_b$.

IV. Remote gating by an external potential

In a molecular system the *physical length* of a side chain is determined by the preparation process. However, the *effective length* can be controlled either by on-site chemical modifications or by an external potential. Here we model the change of the effective chain length by varying continuously the on-site energy of a single terminal site, mimicking the effect of an external local gate potential. The corresponding terminal on-site energy reads, $E_B + eV_g$, while all other on-site energies along the side chain equal E_B . For a small gate potential the on-site energy at the terminal site is resonant with the rest of the sites in the chain and the effective length of the chain is determined by the number of sites. However, when eV_g becomes larger in magnitude than the inter-site hopping matrix elements, the terminal on site energy becomes off resonant from the rest of the chain, and thus the terminal site is effectively decoupled from the chain, which is effectively shortened. This effect of the terminal gate potential can be analyzed using Eqs.(3.11-3.14). The first two steps in the recursion for calculating the relevant Green function for the side chain read in this case,

$$G_{b,1}^{(l)}(E) = \frac{1}{E - E_b - eV_g + i\varepsilon} \xrightarrow{E \rightarrow E_b} \frac{1}{-eV_g + i\varepsilon} \quad (4.1)$$

and,

$$G_{b,2}^{(l)}(E) = \frac{1}{E - E_b + |\gamma_{n,n-1}|^2 / eV_g + i\varepsilon} \xrightarrow{E \rightarrow E_b} \frac{eV_g}{|\gamma_{n,n-1}|^2 + i\varepsilon} \quad (4.2)$$

For $V_g \rightarrow 0$, $G_{b,1}^{(l)}(E)$ diverges and $G_{b,2}^{(l)}(E)$ vanishes, but when $V_g \rightarrow \infty$, $G_{b,1}^{(l)}(E)$ vanishes and $G_{b,2}^{(l)}(E)$ diverges, which is equivalent to starting the recursion from the second site, i.e., the linear chain is effectively shorter by one site.

As an illustrative example, let us focus on the branched conductor sketched in Fig. 3. The electrodes are characterized by the hopping parameter, $\gamma_R = \gamma_L = \gamma_0$. All seven sites of the conductor are associated with the on-site energy, $E_b = 0$, in resonance with the Fermi levels of the two electrodes at zero potential bias. The nearest neighbor hopping matrix elements in the conductor and the hopping matrix elements between the conductor and the electrodes were chosen to be identical and were set to $\gamma = \xi_R = \xi_L = 0.2\gamma_0$. The on-site energy at one of the two terminal sites was set to eV_g modeling the effect of a gate potential.

The zero bias ($V = 0$) transmission function was calculated using Eq.(2.6) for an energy interval around $E \approx E_b = 0$ as a function of V_g . The results presented in Fig. 4, demonstrate that for zero gate voltage, the transmission peaks to unity around $E \approx 0$, but as V_g increases (specifically, as $|eV_g| \gg |\gamma| = 0.2|\gamma_0|$) this transmission peak vanishes. This result is consistent with the change of the effective length of the side chain as analyzed above.

The dependence of the transmission on the effective chain length is reflected directly in the current through the junction. Particularly, in the low temperature and small bias ($T \rightarrow 0, V \rightarrow 0$) limits, the specific characteristics of the conductor are not obscured by

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3 thermal averaging or by the external electrostatic potentials. Defining the chemical
4 potentials at the left and right electrodes for non-zero source-drain bias as $\mu_L = eV/2$
5 and $\mu_R = -eV/2$, and setting the temperature to zero, the current was calculated using
6 Eqs.(2.5,2.6). The results plotted in Fig. 5 demonstrate that in the small bias regime
7 (specifically, when $|eV| < |\gamma| = 0.2 |\gamma_0|$) the current drops from finite values to zero as the
8 magnitude of the terminal gate voltage increases, in accordance with the shortening of the
9 effective terminal chain by one site .
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20 21 22 23 **V. Conclusions**

24 The electronic transport through a branched conductor was analyzed using a simple
25 model within the Landauer transport formulation. It was shown that it is useful to map a
26 branched molecular network onto an effective one dimensional chain, where side
27 branches are represented as local (potential) self energy terms along the main linear
28 chain. On the one hand, this procedure should reduce the complexity of the molecular
29 system under study and particularly it would enable to predict the effect of remote
30 terminal regions on the transport through the conductor. On the other hand, it emphasizes
31 that as in any inverse scattering problem, the experimental observable, i.e. the current
32 through the junction, does not reflect the molecular structure uniquely.
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46 A particularly simple case of a uniform system whose on-site energy is in resonance with
47 the transmitted electrons impact energy was analyzed in detail. In this case the current at
48 a small source-drain potential bias can be switched by changing the length (number of
49 sites) of a "remote" side branch. We demonstrated switching of the current by controlling
50 the "effective length" of a side-chain in terms of an external gate potential.
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3 Future work is required in order to establish the validity of the simple model proposed
4 here for experimentally realizable molecular electronics systems. In particular, effects of
5 electronic correlations, inelastic scattering, electronic nuclear coupling and thermal
6 broadening were ignored within the present model and formulation. However, at least in
7 the coherent quantum regime, it is expected that the transport through a realistic
8 conductor would also be controllable by "remote" modifications in terminal branches, as
9 demonstrated here.
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23
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Figure Captions

Figure 1: Schematic representations of a conducting branched uniform system. The black dots represent electronic sites. Gray dots correspond to discontinuities. (a) The original branched conductor. (b) The effective conductor after eliminating terminal chains of even number of sites. (c) The effective linear conductor after a second elimination step.

Figure 2: Schematic representations of a non-conducting branched uniform system. The black dots represent electronic sites. Gray dots correspond to discontinuities. (a) The original branched conductor. (b) The effective conductor after eliminating terminal chains of even number of sites. (c) The effective linear conductor after a second elimination step.

Figure 3: Schematic representation of a branched uniform conductor. The on-site energy of one of the terminal sites is controlled by a gate potential.

Figure 4: Transmission as a function of the impact electron energy and gate Voltage for a gated branched conductor. Dimensionless units are used.

Figure 5: Current as a function of the source-drain voltage, V , and the terminal gate voltage, V_g , in the small bias regime. Dimensionless units are used.

Figures

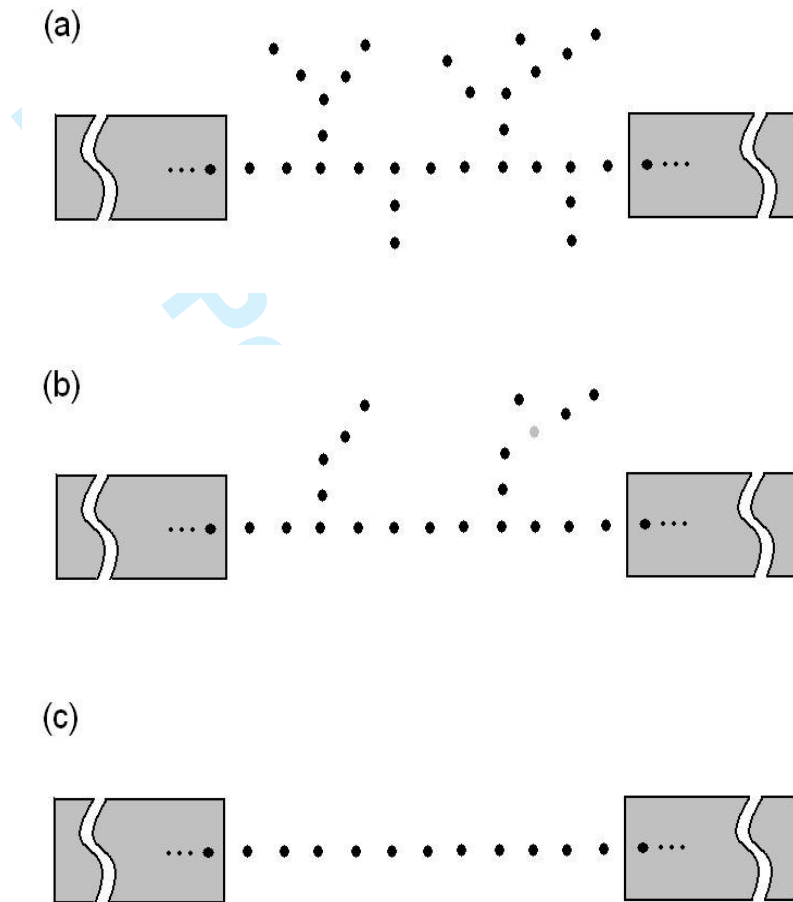


Fig 1

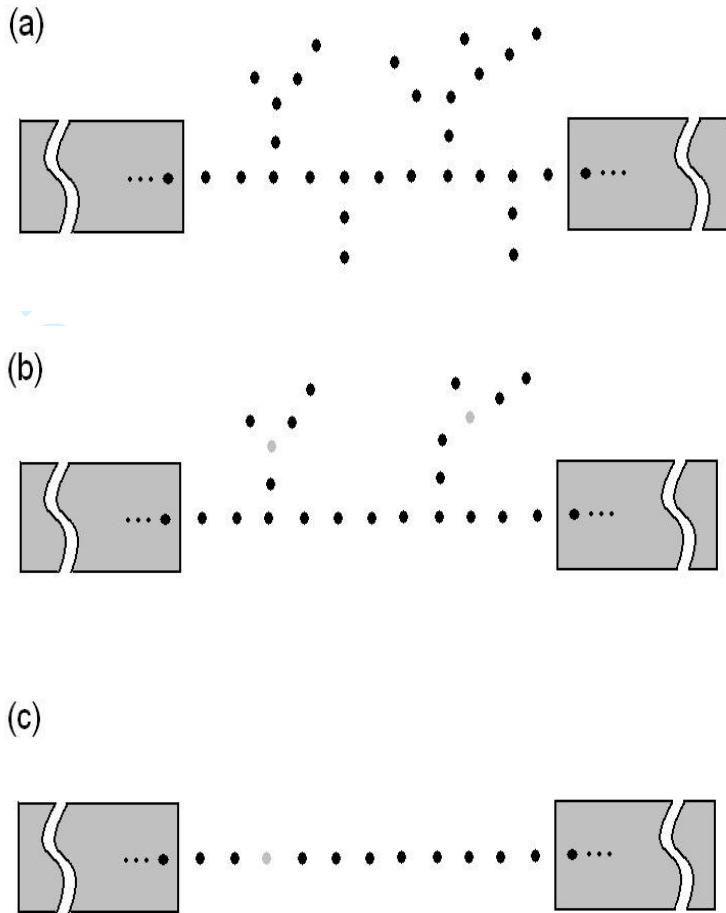


Fig 2

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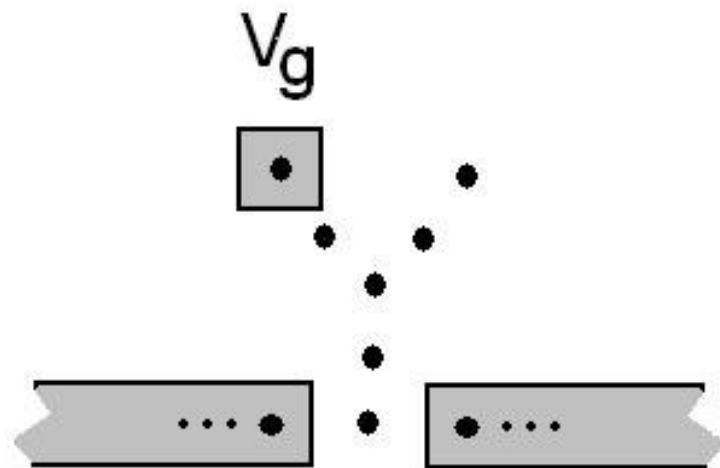


Fig 3

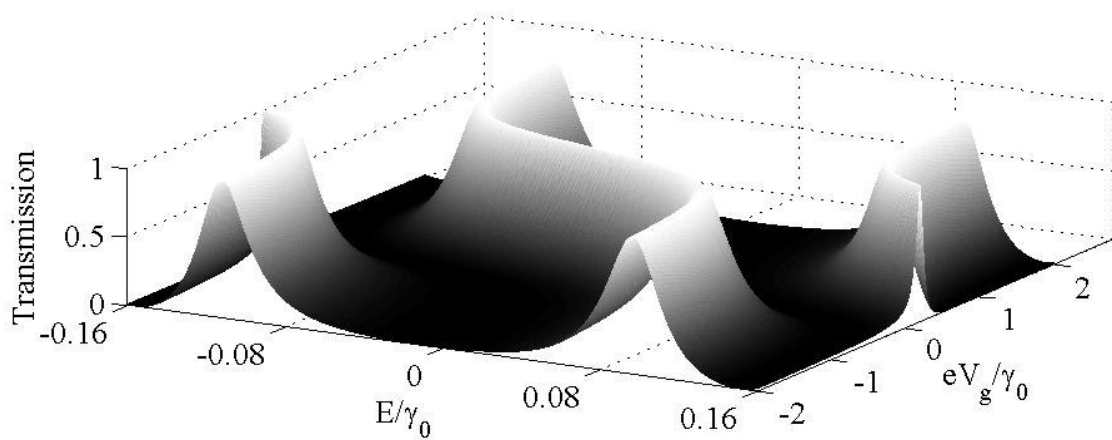


Fig 4

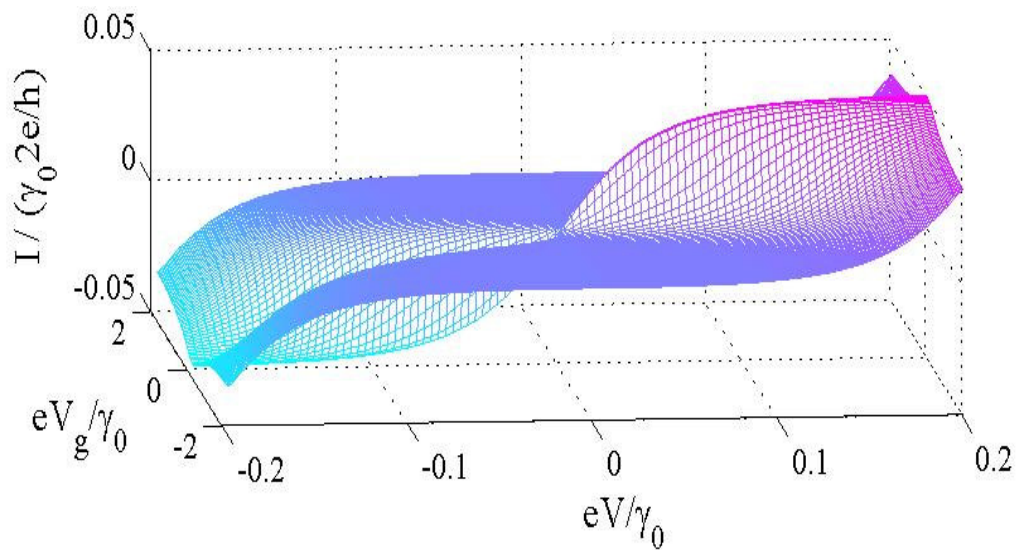


Fig 5

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Controlled Electronic Transport through Branched Molecular Conductors

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Abstract

The conductance through a branched conductor placed between two electrodes is analyzed using the Landauer transport formulation within the framework of the single electron, and the tight binding approximations. Terminal side chains are expressed as self energy terms which map the branched conductor onto an effective linear chain Hamiltonian. The effect of uniform side branches on resonant zero-bias conductance is shown to be analytically solvable and particularly simple, where subtraction or addition of a single terminal site can induce an effective discontinuity in the main linear chain or can effectively decouple the side branch from the conductor. Manipulating the "effective length" of a side branch by a local terminal gate potential, control of the small bias current through the branched conductor is demonstrated.

I. Introduction

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3 In the past decade single molecules were embedded in electrical circuits and the
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5 corresponding electric currents passing through such molecular junctions were
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7 measured[1-7]. Fundamental interest as well as the technological potential of molecular
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9 electronics devices led to rapid progress in this field. Electron transport through a single
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11 molecule is similar in principle to electron transport through quantum dots or wires[8],
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13 but molecular junctions are especially challenging due to the richness of geometrical
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15 structures[7] and configuration changes (electronic-nuclear coupling[9-16]). In particular,
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17 conductors with branched (non linear) molecular structures are most interesting,
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19 suggesting new possibilities for manipulating the transport and for observing new
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21 physical phenomena.
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27 Branched conductors are associated with multiple transmission pathways and the
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29 corresponding interference effects must be accounted for in the coherent transport
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31 regime. Several quantum interference devices were proposed or fabricated in synthetic
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33 two dimensional mesoscopic systems[17] (e.g., the y-branch[18], the T-junction[19], the
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35 dual electron wave coupler[20], the two paths interferometer[21], and quantum dots
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37 arrays[22]). Quantum interference effects in electronic transport through specific pi-
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39 conjugated molecular conductors were also demonstrated theoretically[23-26].
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44 In this work a general formulation is introduced for analyzing the effect of side branches
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46 on the transport through a branched molecular conductor. Single organic molecules[3],
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48 carbon nanotubes[2] or graphene sheets[27,28] provide natural templates for realizations
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50 of such branched molecular systems. The theoretical framework for analyzing the
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52 transport properties is based on the Landauer formulation, invoking a tight binding model
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54 of the electronic system.
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The paper is organized as follows: In section II the model of a branched conductor and the corresponding transport equations are introduced. In section III we show that the conduction through a branched conductor can be formulated in terms of an effective linear chain Hamiltonian. The approach is applied for the simple case of a uniform conductor characterized by constant on-site energies in resonance with the impact electron energy, where the mapping of the branched system onto a linear one is shown to be straight forward. In section IV we demonstrate a conductance switch based on local gating of a remote terminal site of a side branch. Conclusions are given in section V.

II. The branched conductor

Let us consider a branched molecular conductor of the type illustrated in Fig. 1a, invoking a single particle tight binding framework. Each one of N electronic sites is associated with an on-site energy and hopping integrals coupling it to its nearest neighboring sites. The conductor is coupled to two semi-infinite electrodes via two terminal sites. The electrodes are modeled as semi-infinite uniform linear chains, each characterized by a chemical potential and bandwidth, denoted below as μ_L (μ_R) and $4\gamma_L$ ($4\gamma_R$) for the left (right) electrode, respectively. The corresponding hopping integrals between the conductor and the electrodes are denoted below as ξ_L, ξ_R .

Denoting the orthonormal on-site electronic states at the conductor and the J 'th electrode as $|\chi_i^{(c)}\rangle$, and $|\phi_i^{(J)}\rangle$, respectively, the model Hamiltonian is written as follows,

$$\hat{H} = \sum_{J=c,L,R} \hat{H}_J + \sum_{J=L,R} (\hat{H}_{cJ} + \hat{H}_{Jc}), \quad (2.1)$$

where the conductor and the electrodes Hamiltonians are defined as,

$$\hat{H}_c = \sum_{i=1}^N E_i |\chi_i^{(c)}\rangle \langle \chi_i^{(c)}| + \sum_{i,j=1}^N (\gamma_{i,j} |\chi_i^{(c)}\rangle \langle \chi_j^{(c)}| + h.c.) \quad (2.2)$$

$$\hat{H}_J = \sum_{i=1}^{\infty} \mu_J |\varphi_i^{(J)}\rangle \langle \varphi_i^{(J)}| + (\gamma_J |\varphi_i^{(J)}\rangle \langle \varphi_{i+1}^{(J)}| + h.c.) \quad ; \quad J \in R, L \quad (2.3)$$

where $\gamma_{i,j} \neq 0$ only for nearest neighboring sites. The coupling operators between the conductor and the electrodes subspaces are,

$$\begin{aligned} \hat{H}_{cL} &= \xi_L |\chi_1^{(c)}\rangle \langle \varphi_1^{(L)}| \quad ; \quad \hat{H}_{Lc} = \xi_L^* |\varphi_1^{(L)}\rangle \langle \chi_1^{(c)}| \\ \hat{H}_{cR} &= \xi_R |\chi_N^{(c)}\rangle \langle \varphi_1^{(R)}| \quad ; \quad \hat{H}_{Rc} = \xi_R^* |\varphi_1^{(R)}\rangle \langle \chi_N^{(c)}| \end{aligned} \quad (2.4)$$

where the left and right terminal sites of the conductor are associated with $i=1$ and $i=N$ respectively. Using the transport equations of Landauer, the current through the conductor from left to right reads[8],

$$I = \frac{2e}{h} \int_0^{\infty} dE [f_L^e(E) - f_R^e(E)] t(E), \quad (2.5)$$

where $f_J^e(E) = \frac{1}{1 + e^{(E - \mu_J)/k_B T}}$ is the Fermi distribution of electrons at the J'th electrode (assuming only elastic scattering, the holes distributions are not considered explicitly[29]).

The properties of the molecular junction are captured in the transmission function,

$$t(E) = \text{tr}[\hat{\Gamma}_c^{(R)}(E) \hat{G}_c(E) \hat{\Gamma}_c^{(L)}(E) \hat{G}_c^\dagger(E)], \quad (2.6)$$

where the trace is evaluated within the conductor subspace[15]. The corresponding operators $\hat{G}_c(E)$, $\hat{\Gamma}_c^{(L)}(E)$ and $\hat{\Gamma}_c^{(R)}(E)$ are expressed in terms of self energies, defined as,

$$\hat{\Sigma}_J(E) = \lim_{\varepsilon \rightarrow 0} \hat{H}_{cJ} \left[\frac{1}{E - \hat{H}_J + i\varepsilon} \right] \hat{H}_{Jc} \quad ; \quad J = R, L, \quad (2.7)$$

where,

$$\hat{G}_c(E) = \left[E - \hat{H}_c - \hat{\Sigma}_L(E) - \hat{\Sigma}_R(E) \right]^{-1}, \quad (2.8)$$

and

$$\hat{\Gamma}_c^{(J)}(E) = -2 \text{Im}(\hat{\Sigma}_J(E)) \quad ; \quad J = R, L. \quad (2.9)$$

For this model the self energy terms of the left and right electrodes read[15,30],

$$\begin{aligned} \hat{\Sigma}_L(E) &= |\chi_1^{(c)}\rangle\langle\chi_1^{(c)}| \frac{|\xi_L|^2}{2\gamma_L^2} \left[E - \mu_L - i\sqrt{4\gamma_L^2 - (E - \mu_L)^2} \right] ; \quad |E - \mu_L| < 2|\gamma_L| \\ \hat{\Sigma}_R(E) &= |\chi_N^{(c)}\rangle\langle\chi_N^{(c)}| \frac{|\xi_R|^2}{2\gamma_R^2} \left[E - \mu_R - i\sqrt{4\gamma_R^2 - (E - \mu_R)^2} \right] ; \quad |E - \mu_R| < 2|\gamma_R| \end{aligned} \quad (2.10)$$

III. The effective linear chain Hamiltonian

Here we show that within the present model the transport properties (transmission function) of a branched non linear conductor can be mapped exactly on the properties of an effective linear chain. Substituting Eqs.(2.8-2.10) in Eq.(2.6), one can see that the transmission function depends on a single matrix element of the conductor's Green function, i.e.,

$$\hat{G}_{1,N}^{\dagger(c)}(E) = \hat{G}_{N,1}^{(c)}(E) = \langle\chi_N^{(c)}| \left[E - \hat{H}_c - \hat{\Sigma}_L(E) - \hat{\Sigma}_R(E) \right]^{-1} |\chi_1^{(c)}\rangle. \quad (3.1)$$

Let us divide the conductor space into two subspaces, introducing two projection operators[31],

$$\sum_{i=1}^N |\chi_i^{(c)}\rangle\langle\chi_i^{(c)}| = \hat{P}_m + \hat{P}_b \quad ; \quad \hat{P}_m = \sum_{l=1}^m |\chi_l^{(c)}\rangle\langle\chi_l^{(c)}| \quad (3.2)$$

\hat{P}_m projects to a subspace of the conductor which contains m sites ($m \leq N$). This subspace includes the two terminal sites which are coupled to the electrodes ($i_1 = 1$ and

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4 $i_m = N$) and a sequence of electronic sites linking between the terminal sites via a
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6 continuous linear chain. The operator \hat{P}_b projects to the complementary subspace of the
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8 conductor, which contains all the side branches coupled to particular sites along the linear
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10 chain. Using these two projection operators, Eq.(3.1) can be expressed in terms of a
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12 reduced effective Hamiltonian of the linear chain,
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$$15 \quad \hat{G}_{N,1}^{(c)}(E) = \langle \chi_N^{(c)} | [E - \hat{H}_m^{(eff)}]^{-1} | \chi_1^{(c)} \rangle \quad (3.3)$$

$$16 \quad \hat{H}_m^{(eff)} = \hat{H}_m + \hat{\Sigma}_b(E) + \hat{\Sigma}_L(E) + \hat{\Sigma}_R(E), \quad (3.4)$$

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19 where $\hat{\Sigma}_L(E)$ and $\hat{\Sigma}_R(E)$ were defined above (Eq.(2.10)). The Hamiltonian for the
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21 uncoupled linear chain reads,
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$$27 \quad \hat{H}_m = \hat{P}_m \hat{H}_c \hat{P}_m, \quad (3.5)$$

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29 and the coupling to the side branches is captured by another self energy operator,
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$$32 \quad \hat{\Sigma}_b(E) = \lim_{\varepsilon \rightarrow 0} \hat{P}_m \hat{H}_c \hat{P}_b \left[\frac{1}{E - \hat{P}_b \hat{H}_c \hat{P}_b + i\varepsilon} \right] \hat{P}_b \hat{H}_c \hat{P}_m. \quad (3.6)$$

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37 In general, there can be several (up to m) side branches attached to the main linear chain.
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39 For simplicity we assume that each (l 'th) side chain is coupled only to a single site of the
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41 main chain (denoted $|\chi_{i_l}^{(c)}\rangle$) and that the side branches are otherwise decoupled as, e.g.,
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45 in Fig. 1a (the generalization for the more general case is straight forward). $\hat{\Sigma}_b(E)$ can
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47 therefore be conveniently split into additive contributions from the different side
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49 branches,
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$$52 \quad \hat{\Sigma}_b(E) = \sum_{l=1}^M \hat{\Sigma}_b^{(l)}(E)$$

$$\hat{\Sigma}_b^{(l)}(E) = \lim_{\varepsilon \rightarrow 0} \hat{P}_m \hat{H}_c \hat{P}_b^{(l)} \left[\frac{1}{E - \hat{P}_b^{(l)} \hat{H}_c \hat{P}_b^{(l)} + i\varepsilon} \right] \hat{P}_b^{(l)} \hat{H}_c \hat{P}_m \quad (3.7)$$

$\hat{P}_b^{(l)}$ is the projection to the subspace of l 'th side branch, where M is the number of side chains and $\sum_{l=1}^M \hat{P}_b^{(l)} = \hat{P}_b$. Denoting the first on-site state in the corresponding side branch as $|\chi_{j_l}^{(c)}\rangle$, the l 'th self energy term reads,

$$\hat{\Sigma}_b^{(l)}(E) = \sigma_b^{(l)} |\chi_{j_l}^{(c)}\rangle \langle \chi_{j_l}^{(c)}|$$

$$\sigma_b^{(l)}(E) = |\gamma_{i,j_l}|^2 \lim_{\varepsilon \rightarrow 0} \langle \chi_{j_l}^{(c)} | \left[\frac{1}{E - \hat{P}_b^{(l)} \hat{H}_c \hat{P}_b^{(l)} + i\varepsilon} \right] | \chi_{j_l}^{(c)} \rangle. \quad (3.8)$$

Using Eqs.(3.4,3.7,3.8) it follows that the effective Hamiltonian can be written as,

$$\hat{H}_m^{(eff)} = \hat{H}_m(E) + \hat{\Sigma}_L(E) + \hat{\Sigma}_R(E)$$

$$\hat{H}_m(E) = \sum_{l=1}^m (E_{i_l} + \sigma_b^{(l)}(E)) |\chi_{i_l}^{(c)}\rangle \langle \chi_{i_l}^{(c)}| + \sum_{l=2}^m (\gamma_{i_l, i_{l-1}} |\chi_{i_l}^{(c)}\rangle \langle \chi_{i_{l-1}}^{(c)}| + h.c.), \quad (3.9)$$

i.e. the effect of the l 'th side branch amounts to a change ($\sigma_b^{(l)}(E)$) in the on-site (local, potential) energy at the l 'th site of an effectively linear conductor.

Let us focus now on the case of a specific uniform side branch containing a single chain of n sites. By uniform we mean that all on-site energies are identical and equal to E_b (the hopping integral may vary between different sites). The localized states along the side chain are denoted $|\chi_{j_l}^{(c)}\rangle; j_l = 1, 2, \dots, n$, and the coupling to the main chain is via the n 'th site and is denoted $\gamma_{n+1, n}$. The projection operator into the side chain is defined as,

$$\hat{P}_{b,n}^{(l)} = \sum_{j_l=1}^n |\chi_{j_l}^{(c)}\rangle \langle \chi_{j_l}^{(c)}|, \text{ and the (uncoupled) chain Hamiltonian is}$$

$$\hat{P}_{b,n}^{(l)} \hat{H}_c \hat{P}_{b,n}^{(l)} = \sum_{j=1}^n E_b |\chi_{j_i}^{(c)}\rangle \langle \chi_{j_i}^{(c)}| + \sum_{j=2}^n (\gamma_{j_i, j_i-1} |\chi_{j_i}^{(c)}\rangle \langle \chi_{j_i-1}^{(c)}| + h.c.). \quad (3.10)$$

The effect of this side chain on the on-site energy at the main chain can be calculated analytically using the decimation renormalization method[32]. Here we start by expressing the energy-dependent correction to the on-site energy ($\sigma_b^{(l)}(E)$) in terms of the Green operator for the side-chain, using Eq.(3.8),

$$\sigma_b^{(l)}(E) = |\gamma_{n+1,n}|^2 \langle \chi_n^{(c)} | \frac{1}{E - \hat{P}_{b,n}^{(l)} \hat{H}_c \hat{P}_{b,n}^{(l)} + i\varepsilon} | \chi_n^{(c)} \rangle \equiv |\gamma_{n+1,n}|^2 G_{b,n}^{(l)}(E). \quad (3.11)$$

Then we define a hierarchy of projection operators,

$$\hat{P}_{b,n-1}^{(l)} = \hat{P}_{b,n}^{(l)} - |\chi_n^{(c)}\rangle \langle \chi_n^{(c)}|, \quad (3.12)$$

Which are used for constructing recursively the Green operator,

$$G_{b,n}^{(l)}(E) = \frac{1}{E - E_b - |\gamma_{n,n-1}|^2 G_{b,n-1}^{(l)}(E)}. \quad (3.13)$$

The recursion ends at the terminal site ($|\chi_1^{(c)}\rangle$) of the linear side-chain where,

$$G_{b,1}^{(l)}(E) = \lim_{\varepsilon \rightarrow 0} \frac{1}{E - E_b + i\varepsilon}. \quad (3.14)$$

Now let us focus on the case in which the impact electron energy is resonant with the on-site energy along the side chain. As $E \rightarrow E_b$, $G_{b,1}(E)$ diverges, $G_{b,2}(E)$ vanishes and so on, $G_{b,n}(E)$ alternates between infinity and zero as the recursion progresses.

Consequently, $\sigma_b^{(l)}(E)$ diverges for odd number of sites in the side chain (odd n), and vanishes for even values of n . This implies that for $E \rightarrow E_b$ a side chain with an odd number of sites is expressed as an effective local discontinuity in the effective linear conductor, (zero transmission) while a side chain with an even number of sites is

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3 effectively decoupled from the main chain under the same conditions. Notice that the
4 alternations in the transmission due to coupling of a main conductor to a linear side-chain
5 within the tight binding approximation were pointed out before[22,25,26]. These
6 alternations were rightfully attributed to quantum interference between the direct and the
7 indirect scattering pathways.
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11 Our analysis can be further applied when the side branch bifurcates. Consider a side-
12 branch containing a main branch chain, coupled to secondary terminal side chains.
13 Treating these terminal chains according to the above analysis, we conclude that each
14 terminal side-chain can be effectively decoupled from the main branch chain (for an even
15 number of sites) or it can result in an effective discontinuity in the main branch chain (for
16 an odd number of sites). For example, consider the uniform branched conductor with
17 geometry as presented in Fig. 1a for $E \rightarrow E_b$. Eliminating decoupled terminal side-chains
18 or replacing them by discontinuities (according to the corresponding number of sites in
19 each side chain) an effective linear conductor can be obtained recursively, as illustrated in
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39 This analysis suggests that the effective linear conductor Hamiltonian may depend on the
40 number of sites present in a remote side branch, and thus the conductance properties (i.e.
41 the transmission function) may be controlled by manipulating the length of terminal side
42 branches. For demonstration, consider a branched uniform conductor similar to the one
43 presented in Fig. 1 above, but missing one terminal site at the first branch from the left.
44 Repeating our analysis, as illustrated in Fig. 2, one obtains a discontinuity along the
45 effective linear conductor, meaning that in this case, the transmission vanishes for
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56 $E \rightarrow E_b$.
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IV. Remote gating by an external potential

In a molecular system the *physical length* of a side chain is determined by the preparation process. However, the *effective length* can be controlled either by on-site chemical modifications or by an external potential. Here we model the change of the effective chain length by varying continuously the on-site energy of a single terminal site, mimicking the effect of an external local gate potential. The corresponding terminal on-site energy reads, $E_B + eV_g$, while all other on-site energies along the side chain equal E_B . For a small gate potential the on-site energy at the terminal site is resonant with the rest of the sites in the chain and the effective length of the chain is determined by the number of sites. However, when eV_g becomes larger in magnitude than the inter-site hopping matrix elements, the terminal on site energy becomes off resonant from the rest of the chain, and thus the terminal site is effectively decoupled from the chain, which is effectively shortened. This effect of the terminal gate potential can be analyzed using Eqs.(3.11-3.14). The first two steps in the recursion for calculating the relevant Green function for the side chain read in this case,

$$G_{b,1}^{(l)}(E) = \frac{1}{E - E_b - eV_g + i\varepsilon} \xrightarrow{E \rightarrow E_b} \frac{1}{-eV_g + i\varepsilon} \quad (4.1)$$

and,

$$G_{b,2}^{(l)}(E) = \frac{1}{E - E_b + |\gamma_{n,n-1}|^2 / eV_g + i\varepsilon} \xrightarrow{E \rightarrow E_b} \frac{eV_g}{|\gamma_{n,n-1}|^2 + i\varepsilon} \quad (4.2)$$

For $V_g \rightarrow 0$, $G_{b,1}^{(l)}(E)$ diverges and $G_{b,2}^{(l)}(E)$ vanishes, but when $V_g \rightarrow \infty$, $G_{b,1}^{(l)}(E)$ vanishes and $G_{b,2}^{(l)}(E)$ diverges, which is equivalent to starting the recursion from the second site, i.e., the linear chain is effectively shorter by one site.

As an illustrative example, let us focus on the branched conductor sketched in Fig. 3. The electrodes are characterized by the hopping parameter, $\gamma_R = \gamma_L = \gamma_0$. All seven sites of the conductor are associated with the on-site energy, $E_b = 0$, in resonance with the Fermi levels of the two electrodes at zero potential bias. The nearest neighbor hopping matrix elements in the conductor and the hopping matrix elements between the conductor and the electrodes were chosen to be identical and were set to $\gamma = \xi_R = \xi_L = 0.2\gamma_0$. The on-site energy at one of the two terminal sites was set to eV_g modeling the effect of a gate potential.

The zero bias ($V = 0$) transmission function was calculated using Eq.(2.6) for an energy interval around $E \approx E_b = 0$ as a function of V_g . The results presented in Fig. 4, demonstrate that for zero gate voltage, the transmission peaks to unity around $E \approx 0$, but as V_g increases (specifically, as $|eV_g| \gg |\gamma| = 0.2|\gamma_0|$) this transmission peak vanishes. This result is consistent with the change of the effective length of the side chain as analyzed above.

The dependence of the transmission on the effective chain length is reflected directly in the current through the junction. Particularly, in the low temperature and small bias ($T \rightarrow 0, V \rightarrow 0$) limits, the specific characteristics of the conductor are not obscured by thermal averaging or by the external electrostatic potentials. Defining the chemical potentials at the left and right electrodes for non-zero source-drain bias as $\mu_L = eV/2$ and $\mu_R = -eV/2$, and setting the temperature to zero, the current was calculated using Eqs.(2.5,2.6). The results plotted in Fig. 5 demonstrate that in the small bias regime (specifically, when $|eV| \ll |\gamma| = 0.2|\gamma_0|$) the current drops from finite values to zero as the

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3 magnitude of the terminal gate voltage increases, in accordance with the shortening of the
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5 effective terminal chain by one site .
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10 **V. Conclusions**

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12 The electronic transport through a branched conductor was analyzed using a simple
13 model within the Landauer transport formulation. It was shown that it is useful to map a
14 branched molecular network onto an effective one dimensional chain, where side
15 branches are represented as local (potential) self energy terms along the main linear
16 chain. On the one hand, this procedure should reduce the complexity of the molecular
17 system under study and particularly it would enable to predict the effect of remote
18 terminal regions on the transport through the conductor. On the other hand, it emphasizes
19 that as in any inverse scattering problem, the experimental observable, i.e. the current
20 through the junction, does not reflect the molecular structure uniquely.
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34 A particularly simple case of a uniform system whose on-site energy is in resonance with
35 the transmitted electrons impact energy was analyzed in detail. In this case the current at
36 a small source-drain potential bias can be switched by changing the length (number of
37 sites) of a "remote" side branch. We demonstrated switching of the current by controlling
38 the "effective length" of a side-chain in terms of an external gate potential.
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46 Future work is required in order to establish the validity of the simple model proposed
47 here for experimentally realizable molecular electronics systems. In particular, effects of
48 electronic correlations, inelastic scattering, electronic nuclear coupling and thermal
49 broadening were ignored within the present model and formulation. However, at least in
50 the coherent quantum regime, it is expected that the transport through a realistic
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3 conductor would also be controllable by "remote" modifications in terminal branches, as
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5 demonstrated here.
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10 **Acknowledgments**

11
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Figure Captions

Figure 1: Schematic representations of a conducting branched uniform system. The black dots represent electronic sites. Gray dots correspond to discontinuities. (a) The original branched conductor. (b) The effective conductor after eliminating terminal chains of even number of sites. (c) The effective linear conductor after a second elimination step.

Figure 2: Schematic representations of a non-conducting branched uniform system. The black dots represent electronic sites. Gray dots correspond to discontinuities. (a) The original branched conductor. (b) The effective conductor after eliminating terminal chains of even number of sites. (c) The effective linear conductor after a second elimination step.

Figure 3: Schematic representation of a branched uniform conductor. The on-site energy of one of the terminal sites is controlled by a gate potential.

Figure 4: Transmission as a function of the impact electron energy and gate Voltage for a gated branched conductor. Dimensionless units are used.

Figure 5: Current as a function of the source-drain voltage, V , and the terminal gate voltage, V_g , in the small bias regime. Dimensionless units are used.

Figures

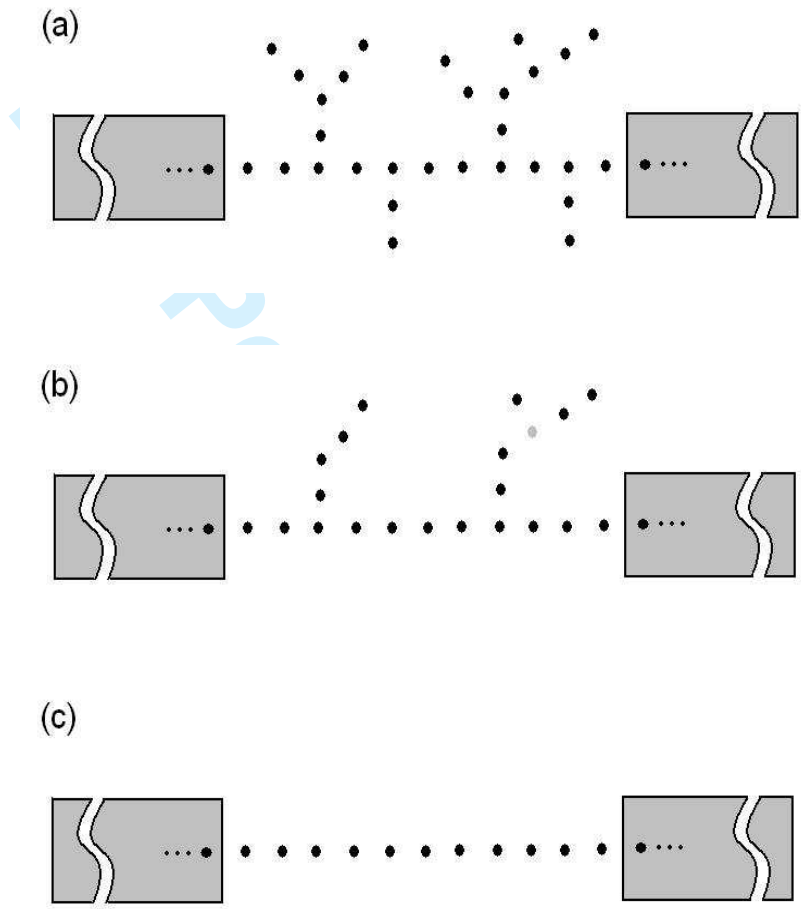


Fig 1

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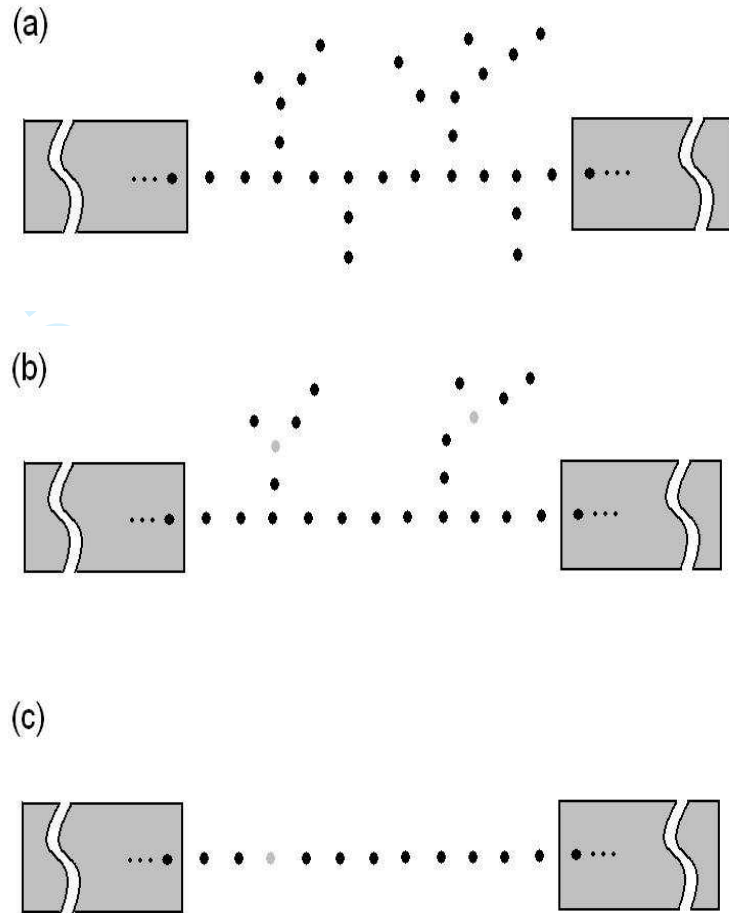


Fig 2

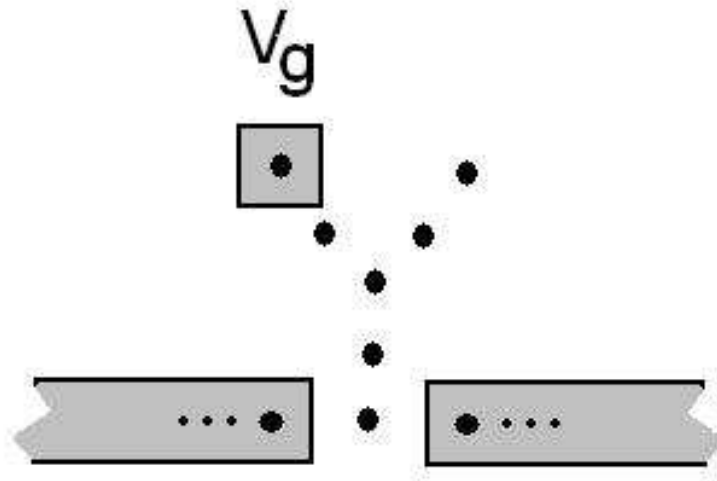


Fig 3

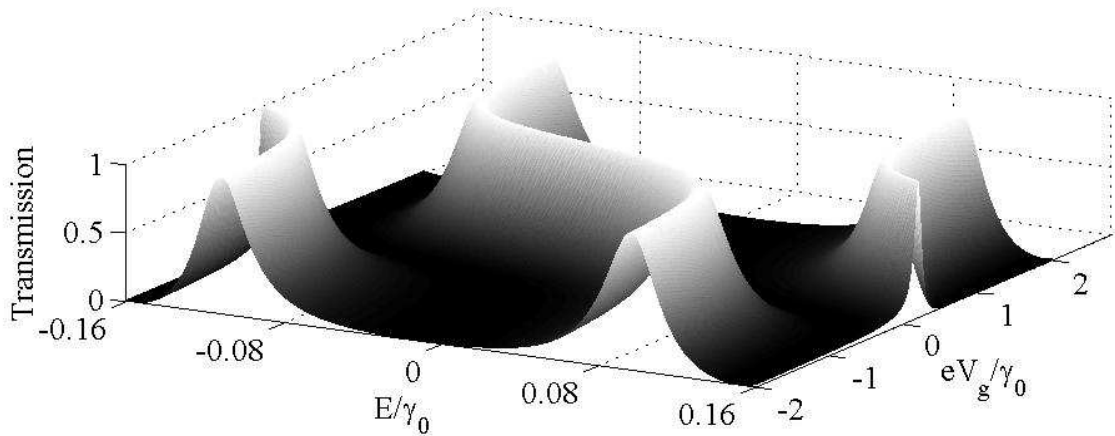


Fig 4

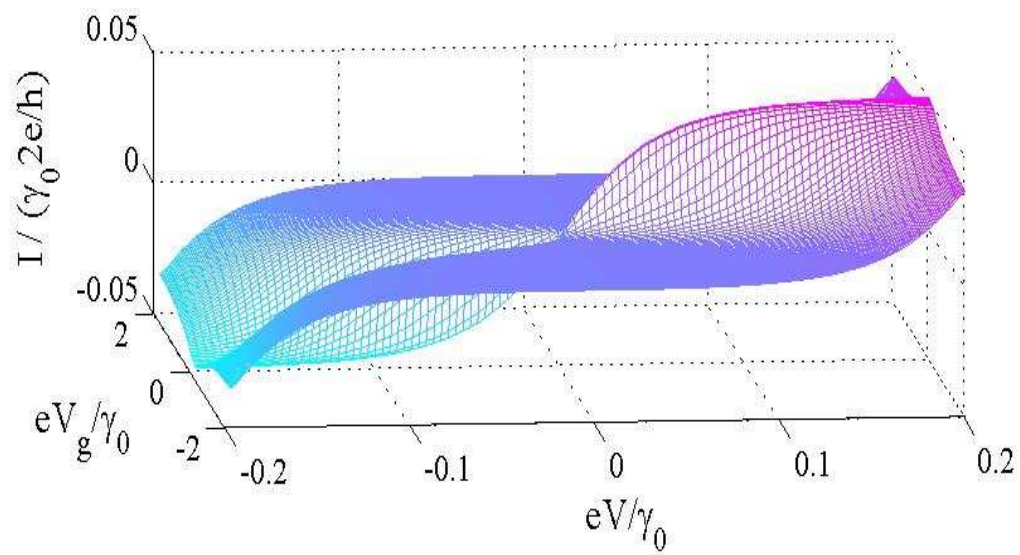
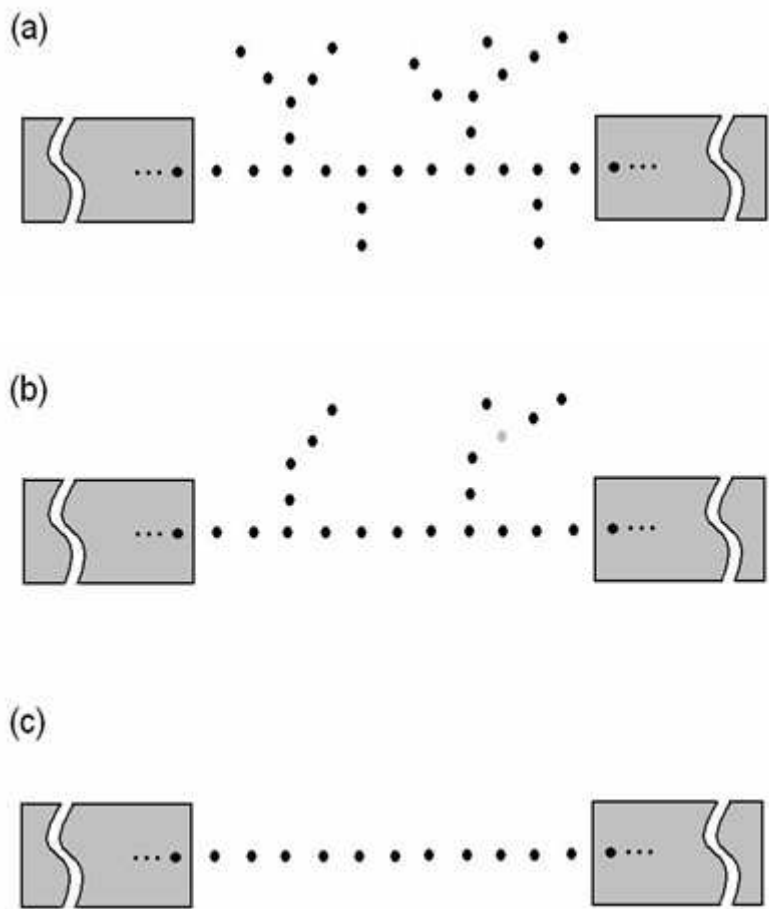


Fig 5

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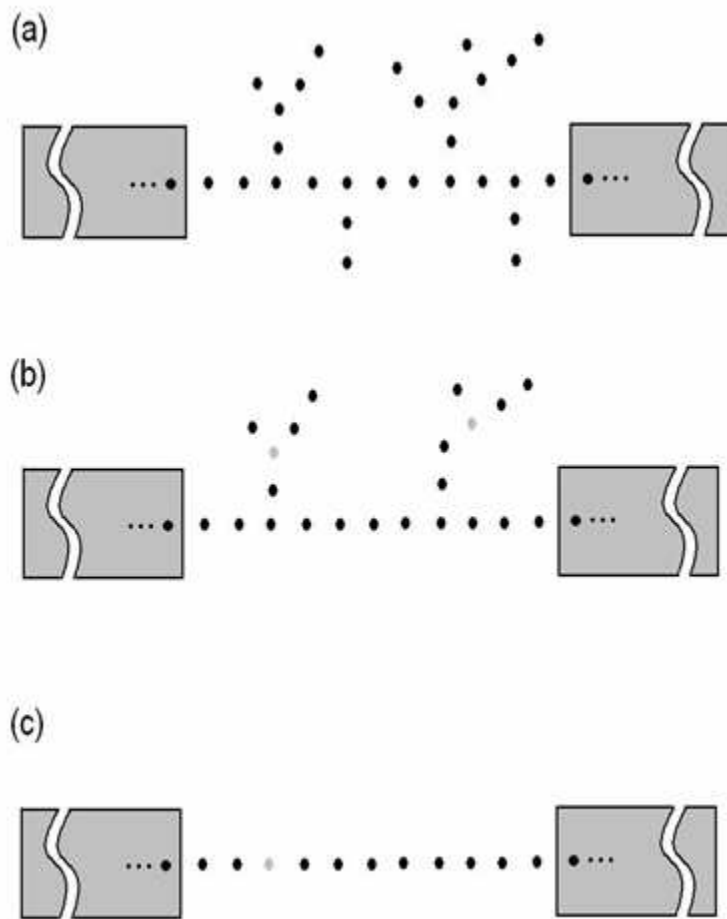
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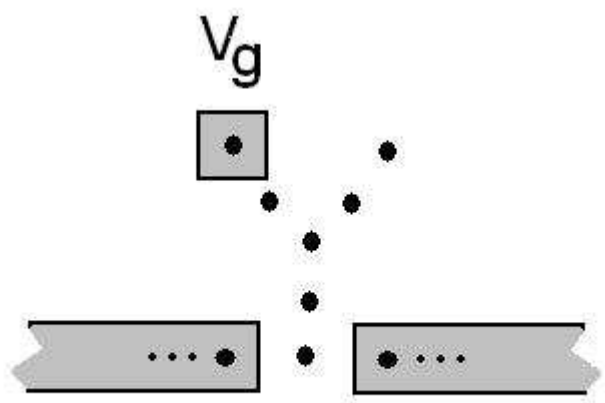
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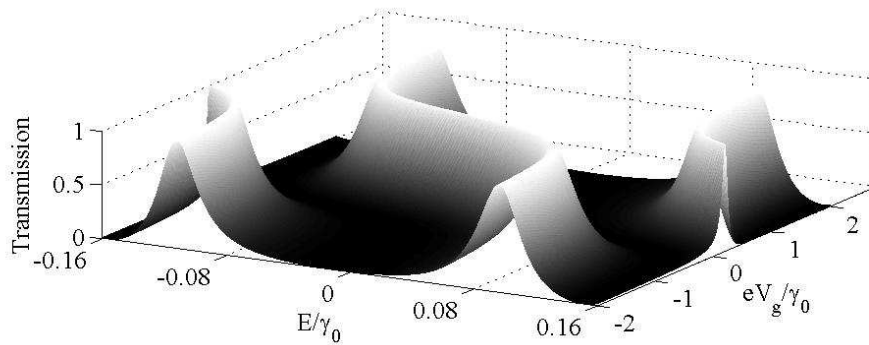
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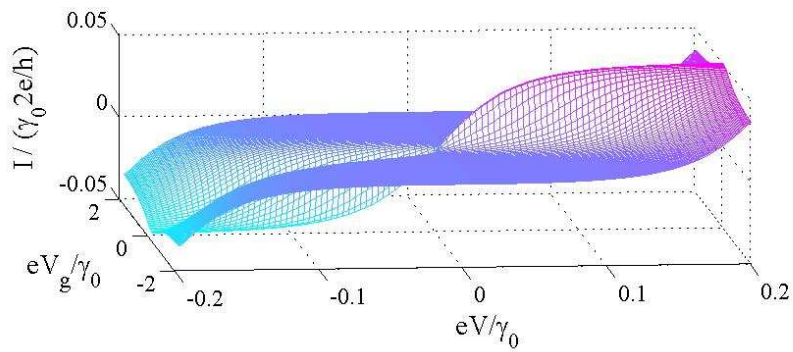
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