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# Transmission properties of coupled atomic wires

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**Abstract.** Electron transmission properties of a configuration consisting of two infinite monatomic chains, which are coupled to each other by either a direct bond or through a finite atomic bridge, are studied via the tight-binding model. A method, based on the multi-channel Lippmann–Schwinger equation, is used to obtain analytical expressions for the $4 \times 4$ scattering matrix, from which transmission probabilities are calculated for several special chain configurations. In particular, we study cases where the bridge is subjected to a constant potential and an electric field, which is generated by a potential difference between the two infinite chains. The results of the theory are very useful for qualitative evaluations of the transmission properties of simple atomic circuits and molecular switches.

## 1. Introduction

The need for improving the operational speed and the integration level of future microelectronic devices places the focus of theoretical research on electron transmission through linear periodic systems at the molecular or atomic level. The study of transmission through periodic molecular chains, containing impurities or defects, provides important insight into the switching properties of conducting polymers, with potential use in molecular electronics. Various configurations of molecular wires, connected to the external world via leads, have been studied [1, 2]. Moreover, techniques, such as manipulation of individual atoms on solid surfaces by a scanning tunnelling microscope [3], or phenomena of spontaneous alignment of atoms on solid surfaces, have opened up prospects of fabrication of periodic atomic chains on insulating substrates. Thus, a study of the transmission properties of various configurations of atomic wires becomes relevant for the design of basic devices such as molecular and atomic switches and memory cells, as well as more complex logic circuits at the atomic level [4].

Electron transmission through molecular and atomic wires is conveniently studied by the tight-binding (TB) model [5, 6, 7, 8] of periodic chains. Describing a polymeric system by a TB hamiltonian with a single orbital per site is certainly an oversimplified model for a molecular-electronic switch. A more adequate use of such a TB model is expected for describing transmission through atomic wires, with the neglect of the coupling to the substrate [4]. However, in both cases TB calculations permit analytical results for transmission coefficients, providing qualitative understanding of modes of switch control in terms of various atomic parameters, which may be related to realistic systems through

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a renormalization approach [9], or via the use of an effective TB hamiltonian [2]. In particular, the TB model is easily handled when one is interested in transmission through more complex configurations of molecule/atom wires involving several leads, such as a T-junction [10, 11].

From the methodological point of view, the transfer-matrix (TM) technique has been used to obtain transmission coefficients for compact, molecular-type, impurities in a host periodic chain [5, 6]. On the other hand, multiple impurities [7] and chains with long-range interactions [8] are handled more easily by the Koster–Slater method [12], based on the Lippmann–Schwinger (LS) equation [13]. Considering chain configurations with multiple leads and extended coupling regions, a multi-channel LS equation approach readily yields the elements of the corresponding scattering matrix. The advantage of the LS method lies in using the asymptotic form of the wave function for the chain configuration to obtain the transmission coefficients, whereas the TM technique would require multiple matrix products of high degree. Moreover, the multi-channel LS approach can be easily extended to TB systems with several orbitals per unit cell.

In section 2, the basic theory for obtaining the $4 \times 4$ scattering matrix (SM) for an H-shaped configuration of atomic wires is presented by solving a multi-channel LS equation. Section 3 is devoted to applications of the theory to various chain configurations derived from the basic H shape. Concluding remarks are given in section 4. Units in which $\hbar = 1$ are used throughout.

## 2. Basic theory

We consider the system, shown in figure 1, which consists of two infinite monatomic chains, $a$ and $c$, interacting with each other by either a direct bond $\eta$ or through a bridge $b$, which connects sites 0 in each chain. Being in constant potential, the chains $a$ and $c$ can both transmit the current. However, their site (bond) energies are, in general, different, $\alpha_a \neq \alpha_c$ ($\beta_a \neq \beta_c$), corresponding to different types of atoms or orbitals, or indicating a possible potential difference $\phi = \alpha_c - \alpha_a$ between the two chains. As a result of the interaction, the energies at sites 0 in both chains are perturbed by changing $\alpha_p$ to $\alpha'_p$ ($p = a, c$). The couplings with the neighbouring sites in both chains, $-1$ and 1, are perturbed in an asymmetric manner, by changing $\beta_p$ to $\gamma_p$ and $\gamma'_p$ ($p = a, c$), respectively. This asymmetry may describe a specific nature of the bonds involved in coupling the chains, but will also be useful in tailoring different chain configurations in subsequent sections. The bridge $b$ consists of a finite, $N$-atom, chain with bond energy $\beta_b$, while site energies $\alpha_b^n$ are labelled by the site position $n = 1, 2, \ldots, N$, to indicate the possibility of having an electric field along the bridge generated by the potential difference $\phi$ between the chains $a$ and $c$. Finally, the bonds between the bridge end atoms 1 and $N$ with the sites 0 in chains $a$ and $c$ are $\mu_a$ and $\mu_c$, respectively, as shown in figure 1.

The transmission properties of such an H-chain configuration are described, in general, by a $4 \times 4$ SM, whose elements will be derived by means of the LS equation. The scattering wave function is represented in asymptotic regions of chains $a$ and $c$ by Bloch waves, $j_p^{-1/2} \exp(\mathrm{i}n\theta_p)$, carrying unit flux, where $j_p = -2\beta_p \sin\theta_p$ is the current through the chain $p$, while the momentum $\theta_p$ is related to the energy $E$, inside the band of the chain $p$ ($= a, c$), via $E = \alpha_p + 2\beta_p \cos\theta_p$. Using matrix notation, the wave function $\mathbf{u}$ is represented by

$$\mathbf{u} = \begin{pmatrix} u_n^a \\ u_n^b \\ u_n^c \end{pmatrix} \tag{1}$$

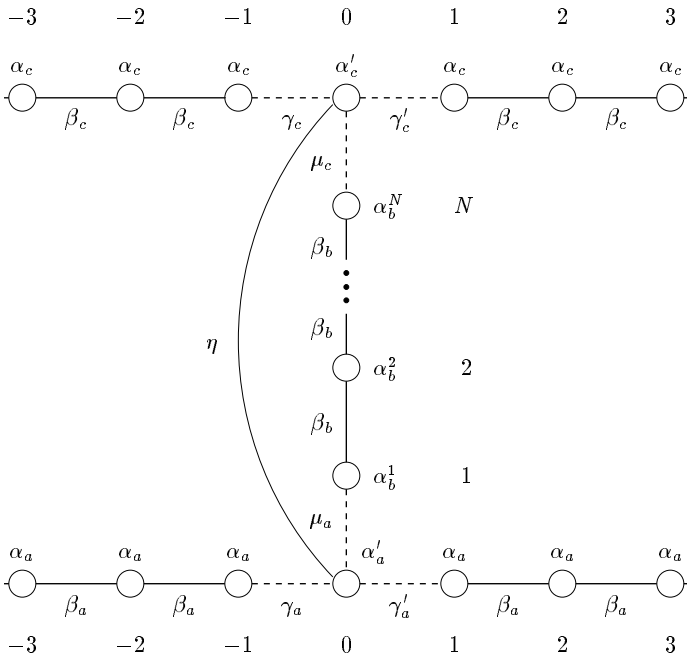


**Figure 1.** Diagram of the basic H chain configuration, for which the scattering matrix elements are evaluated. It is convenient to use the *reduced* quantities: energy $X_p = (E - \alpha_p)/2\beta_p$ (for $p = a, b, c$), site-energy perturbation $Z_p = (\alpha_p' - \alpha_p)/2\beta_p$ and intra-chain bond perturbations $Y_p = \gamma_p/\beta_p$, $Y_p' = \gamma_p'/\beta_p$ (for $p = a, c$), as well as inter-chain bonds $V_a = \mu_a/\sqrt{\beta_a\beta_b}$, $V_c = \mu_c/\sqrt{\beta_c\beta_b}$ and $W = \eta/\sqrt{\beta_a\beta_c}$.

where association of the subscript $n$ with the superscript $p$ in the channel function $u_n^p$ unambiguously restricts $n$ to be a site in the chain $p = a, b, c$. Thus, if the unperturbed wave function represents a Bloch wave, which carries unit current incoming from the left in the chain $a$,

$$\mathbf{u}_0 = \begin{pmatrix} \mathrm{e}^{\mathrm{i}n\theta_a}/\sqrt{j_a} \\ 0 \\ 0 \end{pmatrix} \tag{2}$$

then the scattering wave function will have the form

$$\mathbf{u}_{n\to-\infty} = \begin{pmatrix} \left(\mathrm{e}^{\mathrm{i}n\theta_a} + S_{ll}^{aa}\mathrm{e}^{-\mathrm{i}n\theta_a}\right)/\sqrt{j_a} \\ 0 \\ S_{ll}^{ac}\mathrm{e}^{-\mathrm{i}n\theta_c}/\sqrt{j_c} \end{pmatrix} \tag{3}$$

in far left regions, and

$$\mathbf{u}_{n\to\infty} = \begin{pmatrix} S_{lr}^{aa}\mathrm{e}^{\mathrm{i}n\theta_a}/\sqrt{j_a} \\ 0 \\ S_{lr}^{ac}\mathrm{e}^{\mathrm{i}n\theta_c}/\sqrt{j_c} \end{pmatrix} \tag{4}$$

in far right regions. Here, the elements of the SM have the following meanings: $S_{ll}^{aa}$ is the reflection coefficient for a Bloch wave incoming from the left in chain $a$ and is reflected to the left in chain $a$, $S_{lr}^{aa}$ is the transmission coefficient for a wave going from the left in chain $a$ to the right in chain $a$, $S_{ll}^{ac}$ is the transmission coefficient for a wave coming from the left in chain $a$ to the left in chain $c$ and $S_{lr}^{ac}$ is the transmission coefficient for a wave

going from the left in chain $a$ to the right in chain $c$. All other elements of the SM are, of course, obtained by symmetry. In what follows, we are going to solve the LS equation for the scattering wave function $\mathbf{u}$ and use the asymptotic forms of the channel functions $u_n^a$ and $u_n^c$ to determine the relevant elements of the SM, in conjunction with (3) and (4).

The unperturbed Greenian describes two decoupled infinite chains, $a$ and $c$, and an isolated $N$-atom chain $b$ (a free bridge, possibly placed in an electric field), and is given by the block matrix

$$\mathbf{G}_0 = \begin{pmatrix} g_a(n,k) & 0 & 0 \\ 0 & g_b(n,k) & 0 \\ 0 & 0 & g_c(n,k) \end{pmatrix} \tag{5}$$

where association of $n, k$ with $p$ in $g_p(n,k)$ unambiguously restricts the sites $n$ and $k$ to lie in the chain $p$ ($-\infty < n, k < \infty$ for $p = a, c$ and $1 \leqslant n, k \leqslant N$ for $p = b$). For the *reduced* energy $X_p = \cos\theta_p = (E - \alpha_p)/2\beta_p$ inside the band ($-1 \leqslant X_p \leqslant 1$) of the chain $p = a, c$, the unperturbed Greenian, with the outgoing-wave asymptotic form, can be expressed as [14]

$$g_p(n,k) = \frac{\mathrm{e}^{\mathrm{i}|n-k|\theta_p}}{ij_p} \qquad \text{for } p = a, c \tag{6}$$

where $j_p = -2\beta_p\sqrt{1 - X_p^2}$. The form of the free-bridge Greenian $g_b(n,k)$ will be specified in the following section, which is devoted to applications of the present theory.

Perturbations, describing the interacting system of the figure 1, can be arranged in the $3 \times 3$ block matrix

$$\mathbf{V} = \begin{pmatrix} V_{km}^{aa} & V_{km}^{ab} & V_{km}^{ac} \\ V_{km}^{ba} & V_{km}^{bb} & V_{km}^{bc} \\ V_{km}^{ca} & V_{km}^{cb} & V_{km}^{cc} \end{pmatrix} = \begin{pmatrix} V_{km}^{aa} & \mu_a\delta_{k0}\delta_{m1} & \eta\delta_{k0}\delta_{m0} \\ \mu_a\delta_{k1}\delta_{m0} & 0 & \mu_b\delta_{kN}\delta_{m0} \\ \eta\delta_{k0}\delta_{m0} & \mu_b\delta_{k0}\delta_{mN} & V_{km}^{cc} \end{pmatrix} \tag{7}$$

where

$$V_{km}^{pp} = (\alpha_p' - \alpha_p)\delta_{k0}\delta_{m0} + (\gamma_p - \beta_p)(\delta_{k0}\delta_{m,-1} + \delta_{k,-1}\delta_{m0}) + (\gamma_p' - \beta_p)(\delta_{k0}\delta_{m1} + \delta_{k1}\delta_{m0}), \tag{8}$$

for $p = a, c$. Note that the explicit form of the perturbation matrix, (7) with (8), given in terms of Kronecker deltas, is based on the convention that $V_{km}^{pq}$ describes a perturbation involving site $k$ in chain $p$ and site $m$ in chain $q$, where $p, q = a, b, c$.

Finally, the multi-channel LS equation,

$$\mathbf{u} = \mathbf{u}_0 + \mathbf{G}_0\mathbf{V}\mathbf{u} \tag{9}$$

with the unperturbed solution (2), can be written in the following component form

$$u_n^a = \frac{\mathrm{e}^{\mathrm{i}n\theta_a}}{\sqrt{j_a}} + (\alpha_a' - \alpha_a)g_a(n,0)u_0^a + (\gamma_a - \beta_a)\left[g_a(n,0)u_{-1}^a + g_a(n,-1)u_0^a\right] + (\gamma_a' - \beta_a)\left[g_a(n,0)u_1^a + g_a(n,1)u_0^a\right] + \mu_a g_a(n,0)u_1^b + \eta g_a(n,0)u_0^c \tag{10}$$

$$u_n^b = \mu_a g_b(n,1)u_0^a + \mu_c g_b(n,N)u_0^c \tag{11}$$

$$u_n^c = (\alpha_c' - \alpha_c)g_c(n,0)u_0^c + (\gamma_c - \beta_c)\left[g_c(n,0)u_{-1}^c + g_c(n,-1)u_0^c\right] + (\gamma_c' - \beta_c)\left[g_c(n,0)u_1^c + g_c(n,1)u_0^c\right] + \mu_c g_c(n,0)u_N^b + \eta g_c(n,0)u_0^a. \tag{12}$$

After some algebra, it is possible to express the solution for the channel functions in chains $a$ and $c$ in compact form, in terms of $u_0^a$ and $u_0^c$, as follows

$$u_n^p = v_n^p + \left(u_0^p - v_0^p\right)\frac{g_p(n,0)}{g_p(0,0)} + \left\{(\gamma_p - \beta_p)\left[g_p(n,-1) - g_p(n,0)\mathrm{e}^{\mathrm{i}\theta_p}\right] + (\gamma_p' - \beta_p)\left[g_p(n,1) - g_p(n,0)\mathrm{e}^{\mathrm{i}\theta_p}\right]\right\}u_0^p \tag{13}$$

with $p = a, c$, where

$$v_n^a = \frac{\mathrm{e}^{\mathrm{i}n\theta_a}}{\sqrt{j_a}} + g_a(n,0)\left[\eta + \mu_a\mu_c g_b(1,N)\right]u_0^c \tag{14}$$

$$v_n^c = g_c(n,0)\left[\eta + \mu_c\mu_a g_b(N,1)\right]u_0^a. \tag{15}$$

Explicit forms of $u_0^a$ and $u_0^c$ are readily obtained by solving the coupled equations

$$u_0^p = \frac{1}{D_p}\left\{\left[2X_p - (Y_p + Y_p')\mathrm{e}^{\mathrm{i}\theta_p}\right]v_0^p + (Y_p - 1)v_{-1}^p + (Y_p' - 1)v_1^p\right\} \qquad p = a, c \tag{16}$$

in conjunction with (14) and (15), where

$$D_a = 2(X_a - Z_a) - \left[Y_a^2 + (Y_a')^2\right]\mathrm{e}^{\mathrm{i}\theta_a} - V_a^2\widetilde{g}_b(1,1) \tag{17}$$

$$D_c = 2(X_c - Z_c) - \left[Y_c^2 + (Y_c')^2\right]\mathrm{e}^{\mathrm{i}\theta_c} - V_c^2\widetilde{g}_b(N,N). \tag{18}$$

Here, we have used reduced quantities $Y_p = \gamma_p/\beta_p$, $Y_p' = \gamma_p'/\beta_p$, $Z_p = (\alpha_p' - \alpha_p)/2\beta_p$, and $V_p = \mu_p/\sqrt{\beta_p\beta_b}$ for $p = a, c$. Note that the Greenian of the bridge $b$ is now expressed in a reduced form $\widetilde{g}_b(n,m) \equiv \beta_b g_b(n,m)$.

Taking $n \to \pm\infty$ in (13) and comparing with (3) and (4) yields the SM elements

$$S_{ll}^{aa} = -1 - 2\mathrm{i}\sqrt{1 - X_a^2}\,Y_a^2\frac{D_c}{\Delta} \tag{19}$$

$$S_{lr}^{aa} = -2\mathrm{i}\sqrt{1 - X_a^2}\,Y_a Y_a'\frac{D_c}{\Delta} \tag{20}$$

$$S_{ll}^{ac} = -2\mathrm{i}\left[(1 - X_a^2)(1 - X_c^2)\right]^{1/4} Y_a Y_c\frac{C_{ca}}{\Delta} \tag{21}$$

$S_{lr}^{ac}$ being obtained from (21) simply by replacing $Y_c$ by $Y_c'$. Here, $\Delta = D_a D_c - C_{ac}C_{ca}$, with

$$C_{ac} = W + V_a V_c\widetilde{g}_b(1,N)$$
$$C_{ca} = W + V_c V_a\widetilde{g}_b(N,1) \tag{22}$$

where we define $W = \eta/\sqrt{\beta_a\beta_c}$. It should be noted that, in the definitions (17) and (18) of $D_a$ and $D_c$, one has to specify analytic continuation of the factors $\mathrm{e}^{\mathrm{i}\theta_p}$ outside the band of chain $p = a, c$, namely

$$\mathrm{e}^{\mathrm{i}\theta_p} = \begin{cases} X_p + i\sqrt{1 - X_p^2} & \text{for } |X_p| \leqslant 1 \\ X_p - \mathrm{sign}(X_p)\sqrt{X_p^2 - 1} & \text{for } |X_p| > 1. \end{cases} \tag{23}$$

Equations (19) to (21), together with the definitions (17), (18), (22) and (23), constitute the main results of the present theory. Transmission probabilities are obtained as squared moduli of the corresponding SM elements (19) to (21), with the final remarks that $S_{ll}^{aa}$ and $S_{lr}^{aa}$ are nonzero for $|X_a| \leqslant 1$, while $S_{ll}^{ac}$ and $S_{lr}^{ac}$ are nonzero for $|X_a| \leqslant 1$ *and* $|X_c| \leqslant 1$, that is, for energies $E$ inside the band overlap region of the chains $a$ and $c$.

## 3. Applications

In this section, we study the transmission properties of specific chain configurations, which can be tailored from the basic H configuration of figure 1 by using convenient choices for the various coupling parameters. Note that the reduced quantities are listed, for convenience, in the caption of figure 1.

### *3.1. Directly coupled infinite chains*

We consider here the transmission properties of two identical chains, which are coupled by the bond $W$, connecting the chains' sites 0. The bridge is removed by taking $V_a = V_c = 0$, and we take $X_a = X_c \equiv X$, $Y_a = Y'_a = Y_c = Y'_c = 0.5$ and $Z_a = Z_c = 0$. We have plotted in figure 2 the $X$ and $W$ dependences of the chain-$a$ reflection probability (a), chain-$a$ transmission probability (b) and chain-$c$ transmission probabilities (c). Of course, the plots add up to unity over the whole $(X, W)$ region.

### *3.2. Loop*

Another configuration, of some interest for a memory cell [4], is an $(N+1)$-atom loop [10] of a chain, which can be generated by taking the bridge $b$ in constant potential and assuming that it is made of same material as chain $a$ ($\alpha_b^n = \alpha_a$ for $n = 1, \ldots, N$ and $\beta_b = \beta_a$). The loop is formed by taking $Y_c = Y'_c = 0$, $Z_c = 0$, $V_c = 1$ and $W = Y_a = Y'_a = V_a \equiv Y$. Transmission probability through the loop is obtained from $|S_{lr}^{aa}|^2$ and is nonzero for energies $X_a \equiv X$ inside the band of chain $a$ ($|X| \leqslant 1$). Then, the elements of the bridge Greenian, required in $S_{lr}^{aa}$, can expressed in terms of Chebyshev polynomials $U_n(X)$, as follows

$$\begin{aligned} \widetilde{g}_b(1,1) &= \widetilde{g}_b(N,N) = U_{N-1}(X)/U_N(X) \\ \widetilde{g}_b(1,N) &= \widetilde{g}_b(N,1) = 1/U_N(X). \end{aligned} \tag{24}$$

The $X$ and $Y$ dependence of the loop transmission probability is plotted in figure 3 for $N + 1 = 5$ and $Z_a = 0$. An interesting feature is the exact vanishing of the transmission probability at the band centre, due to existence of a local antiresonance [10].

### *3.3. T-junction in constant potential*

A T-junction with three semi-infinite leads [11] is obtained simply by taking $V_a = V_c = Y_c = 0$ and $Y'_c = 1$, $Z_c = 0$. We shall assume that the chain $a$ is not perturbed ($X_a \equiv X$, $Y_a = Y'_a = 1$ and $Z_a = 0$) and that the remaining half of the chain $c$ has $\alpha_c = \alpha_a$ and $\beta_c = R\beta_a$, so that, $X_c = X/R$. The $X$ and $W$ dependence of transmission probability through the chain $a$ is plotted in figure 4(a) for $R = 0.5$.

The case of one lead being a finite [10], $N$-atom chain, is generated by taking $W = V_c = 0$. We have, in fact, the bridge $b$ adsorbed on the site 0 of the chain $a$ (which we take as unperturbed, $X_a \equiv X$, $Y_a = Y'_a = 1$, $Z_a = 0$) via the bond $V_a \equiv V$. In the transmission probability $|S_{lr}^{aa}|^2$, we need the bridge Greenian element $\widetilde{g}_b(1,1)$, analytically continued outside the bridge band,

$$\widetilde{g}_b(1,1) = \begin{cases} \dfrac{U_{N-1}(X_b)}{U_N(X_b)} & \text{for } |X_b| \leqslant 1 \\ \operatorname{sign}(X_b)\dfrac{\sinh\left[N\operatorname{arccosh}\left(|X_b|\right)\right]}{\sinh\left[(N+1)\operatorname{arccosh}\left(|X_b|\right)\right]} & \text{for } |X_b| > 1. \end{cases} \tag{25}$$

Taking $\alpha_b^n = \alpha_a$ and $\beta_b = R\beta_a$, that is, $X_b = X/R$, we plot the $X$ and $V$ dependence of transmission probability in figure 4(b) for $N = 4$ and $R = 0.5$. The effect of the adsorbed $N$-atom branch on the host chain is seen to introduce $N$ (=4 for $R < 1$) dips in the transmission probability, as the adsorption bond $V$ increases.

### *3.4. T-junction in electric field*

A T-junction with one, semi-infinite, lead in an electric field is obtained by taking $W = V_c = 0$, and placing the semi-infinite bridge in an electric field of gradient $\Gamma$, so

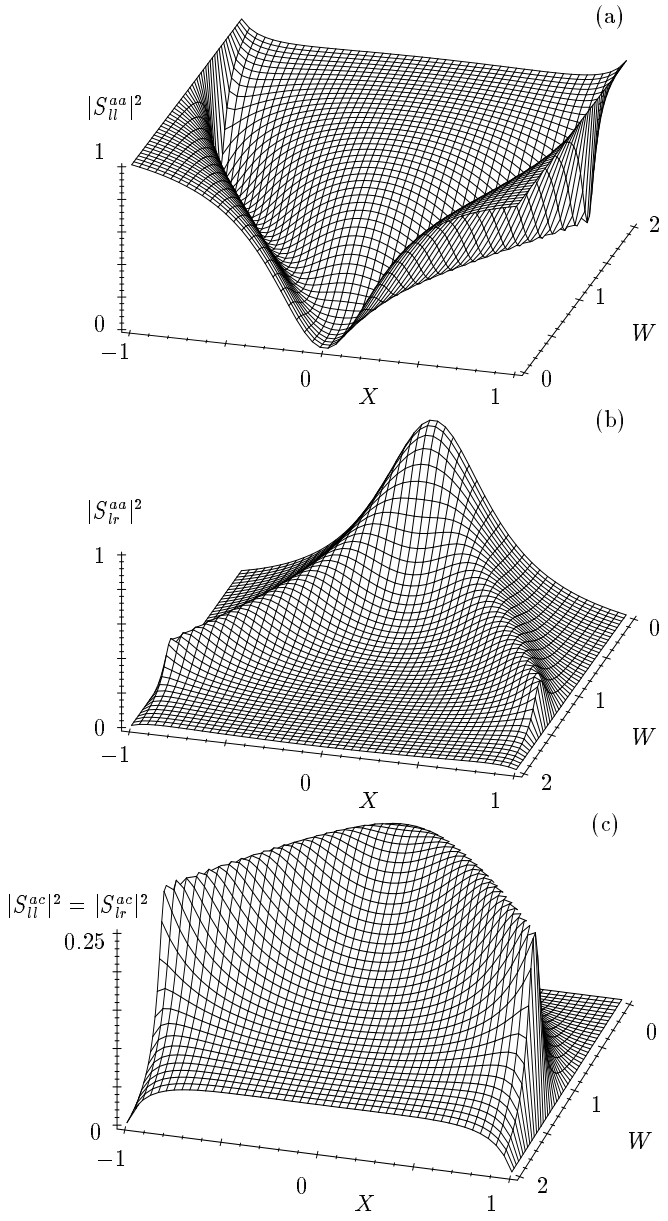


**Figure 2.** Dependence of the transmission through two identical chains on energy $X$ and inter-chain coupling $W$: chain-$a$ reflection probability (a), chain-$a$ transmission probability (b) and chain-$c$ transmission probabilities (c).

that $\alpha_b^n = \alpha_b^1 + (n-1)\Gamma$ for $1 \leqslant n < \infty$. The bridge Greenian, needed in $S_{lr}^{aa}$, is given by [15]

$$\widetilde{g}_b(1,1) = \mathrm{sign}(F_b)\frac{J_{-\xi}\left(|F_b|^{-1}\right)}{J_{-\xi-1}\left(|F_b|^{-1}\right)} \tag{26}$$

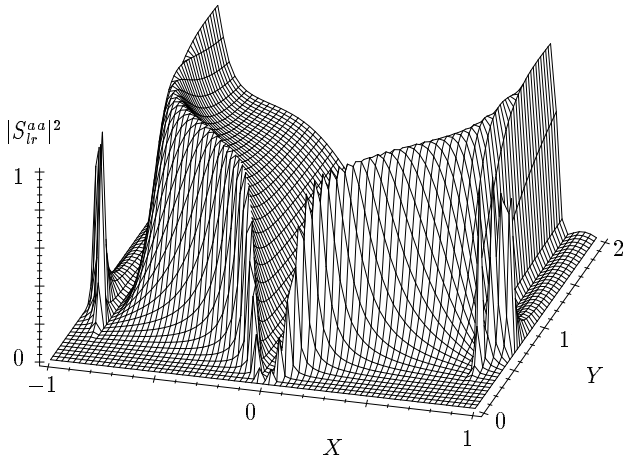


**Figure 3.** Dependence of the transmission probability through a chain with $N+1=5$-atom loop on energy $X$ and bonds $Y$ of the crossing site.

where $J$ is the Bessel function of the first kind, $F_b = \Gamma/2\beta_b$, and $\xi = X_b/F_b$ with $X_b = (E-\alpha_b^1)/2\beta_b$. Taking again the chain $a$ to be unperturbed ($X_a \equiv X$, $Y_a = Y_a' = 1$ and $Z_a = 0$), we define $F = \Gamma/2\beta_a = RF_b$, where $R = \beta_b/\beta_a$. Moreover, assuming $\alpha_b^1 = \alpha_a$, we have $X_b = X/R$. The dependence of the transmission probability through the chain $a$ on $X$ and $V \equiv V_a$ is plotted in figure 5(a) for $F = 0.15$ and $R = 0.5$. Again, dips in the transmission probability of the host chain reflect the local (discrete) density of states at the site 1 of the lead in the field [15]. Figure 5(b) presents just the cross-sections of the plot in figure 5(a), for $V = 0.5$ and $V = 1.5$, which reveal more detailed features of the transmission probability.

### *3.5. Sandwich in constant potential and electric field*

A sandwich structure [16, 17] consists of a finite, $N$-atom chain between two semi-infinite leads of same material, and is obtained by taking $W = Y_a' = Y_c = 0$, as well as $Y_a = Y_c' = 1$, $Z_a = Z_c = 0$. When the bridge is placed in a constant potential and coupled to the leads by $V_a = V_c \equiv V$, its Greenian elements $\widetilde{g}_b(1,1) = \widetilde{g}_b(N,N)$ are both given by the definition (25). Similarly, the cross elements $\widetilde{g}_b(1,N) = \widetilde{g}_b(N,1)$, required in $S_{lr}^{ac}$, are given by

$$\widetilde{g}_b(1,N) = \begin{cases} \dfrac{1}{U_N(X_b)} & \text{for } |X_b| \leqslant 1 \\ \big[\operatorname{sign}(X_b)\big]^N \dfrac{\sqrt{X_b^2-1}}{\sinh\left[(N+1)\operatorname{arccosh}(|X_b|)\right]} & \text{for } |X_b| > 1. \end{cases} \tag{27}$$

Assuming $\alpha_a = \alpha_b = \alpha_c$ and $\beta_a = \beta_c = \beta_b/R$, we have $X_a = X_c \equiv X$ and $X_b = X/R$. The $X$ and $V$ dependence of the transmission probability through the sandwich in a constant potential, $|S_{lr}^{ac}|^2$, is plotted in figure 6(a) for $N = 4$ and $R = 0.5$. Thus, we have an $N$-atom impurity, immersed in a host chain, which shows up in the transmission probability as series of resonance peaks, for sufficiently weak adsorption bond $V$.

A sandwich in an electric field is represented by two semi-infinite leads (obtained by $W = Y_a' = Y_c = 0$, as well as $Y_a = Y_c' = 1$, $Z_a = Z_c = 0$), placed in constant, but different, potentials, with potential difference $\phi$. Assuming that $\alpha_c = \alpha_b^N = \alpha_a + \phi = \alpha_b^1 + \phi$,

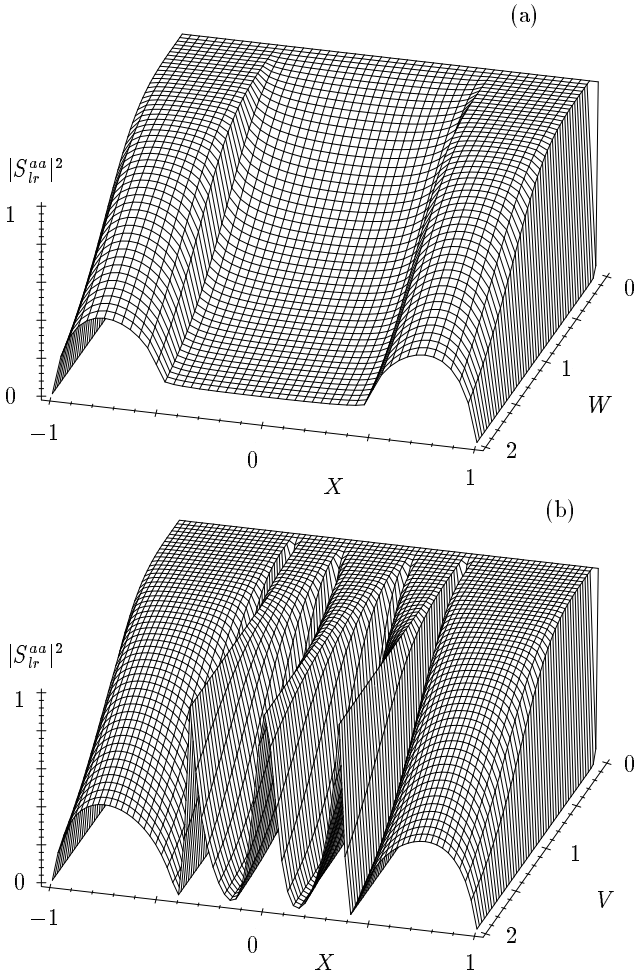


**Figure 4.** Transmission probability through a T-junction in constant potential, with the ratio of band widths $R = 0.5$, versus energy $X$ and bonds $W$ or $V$ for: three semi-infinite leads (a), and one lead being $N = 4$-atom branch adsorbed on the chain $a$ (b).

we have the field gradient across the $N$-atom bridge $\Gamma = \phi/(N-1)$. Assuming further that $\beta_a = \beta_c$, we have $X_c = X_a - 2U$, where $U = \phi/4\beta_a$ is the reduced potential difference between the leads, so that the transmission probability $|S_{lr}^{ac}|^2$ is non-zero for non-vanishing band-overlap between the leads, defined by $0 \leqslant U < 1$. Defining the field strength by $F = \Gamma/2\beta_a = 2U/(N-1)$, we have $F_b = F/R$, where $R = \beta_b/\beta_a$. Referring to $X_b = (E - \alpha_b^1)/2\beta_b = X_a/R$ as the reduced energy at the site 1 of the bridge and $X_b' = (E - \alpha_b^N)/2\beta_b = X_b - (N-1)F_b$ as the reduced energy at the site $N$ of the bridge, we define $\xi = X_b/F_b = X_a/F$ and $\xi' = X_b'/F_b = \xi - N + 1$. The relevant Greenian elements may now be written as [17]

$$\widetilde{g}_b(1,1) = -\frac{Y_{-\xi}J_{-\xi'+1} - J_{-\xi}Y_{-\xi'+1}}{Y_{-\xi-1}J_{-\xi'+1} - J_{-\xi-1}Y_{-\xi'+1}} \tag{28}$$

$$\widetilde{g}_b(N,N) = \frac{Y_{\xi'}J_{\xi+1} - J_{\xi'}Y_{\xi+1}}{Y_{\xi'-1}J_{\xi+1} - J_{\xi'-1}Y_{\xi+1}} \tag{29}$$

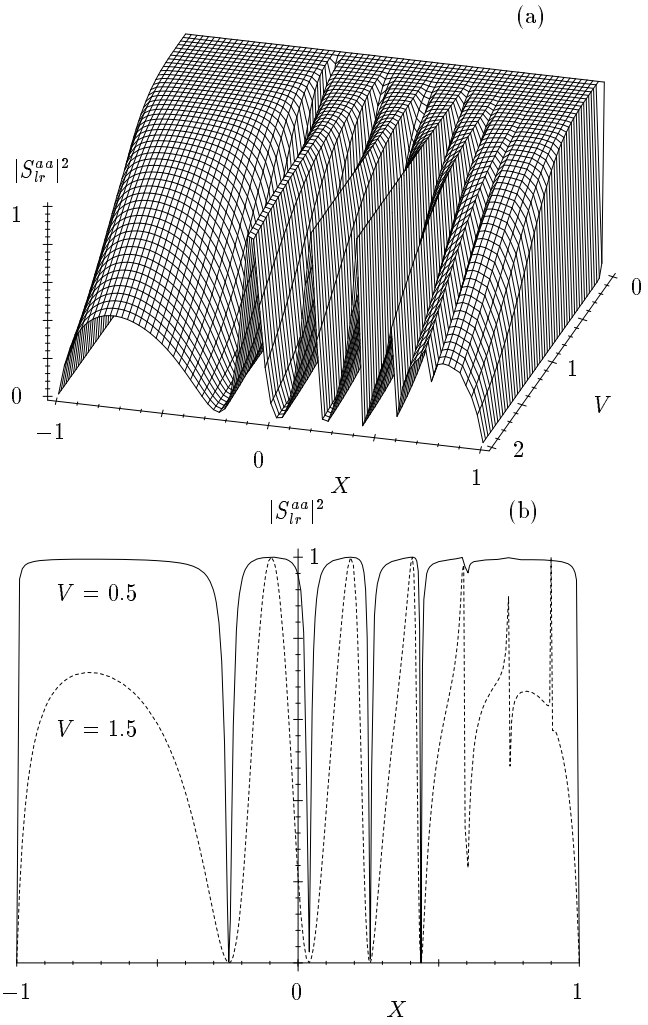


**Figure 5.** Transmission probability through a T-junction, with one lead in electric field $F = 0.15$ and the ratio of band widths $R = 0.5$, versus energy $X$ and bond $V$ (a). Fine structure of the transmission is shown for $V = 0.5$ and $V = 1.5$ (b).

$$\widetilde{g}_b(1, N) = \widetilde{g}_b(N, 1) = \frac{\dfrac{2F}{\pi R}}{Y_{-\xi-1}J_{-\xi'+1} - J_{-\xi-1}Y_{-\xi'+1}} \tag{30}$$

where the Bessel functions of the first (second) kind $J$ ($Y$) depend on $1/F_b$. Transmission probability through the sandwich in the electric field is plotted in figure 6(b) for U=0.5 (the overlapping region of the chain-$a$ band is then $0 \leqslant X_a \leqslant 1$), and $N = 10$ and $R = 0.5$, as a function of the coupling to the leads, $V_a = V_b \equiv V$. The transmission probability shows a number of resonant peaks, reflecting a portion of a quasi-Wannier–Stark ladder [15, 17], formed in the bridge.

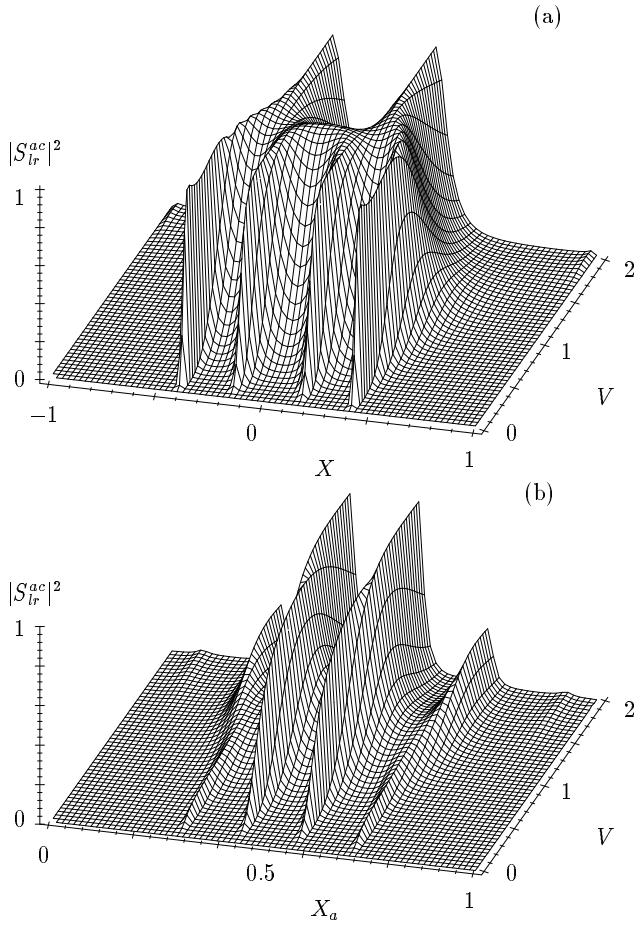


**Figure 6.** Dependence of the transmission through sandwich on energy $X$ and bond $V$ for bandwidth ratio $R = 0.5$: $N = 4$-atom sandwich in constant potential (a), $N = 10$-atom sandwich in the field, generated by the $U = 0.5$ potential difference between the leads (b).

## 4. Concluding remarks

The theory of section 2 provides simple analytical expressions for the SM elements of the basic H structure of figure 1 in terms of the bridge Greenian elements and a number of perturbed site and bond energies. These results may prove useful for quick qualitative estimates of transmission properties of a number of chain configurations, as described in section 3. Special attention has been given to the cases with a bridge in an electric field, for which the relevant Greenian elements can expressed in an analytical manner in terms of Bessel functions. In this way we provide an analytical tool for studying basic elements of atomic-wire circuits. For example, taking $W = 0$ in the H configuration of figure 1, provides a model for a prototype atomic relay [4] by placing the feed line $c$ in a potential, so that the field across the bridge $b$ may be used to control the transmission through the chain $a$ by displacing the atom at the site 0, thus weakening the bonds to its neighbours at sites $-1$ and 1. Finally, let us mention that one can analyse the switching times, related to the various transmission channels in the H structure by a straightforward extension of our

study of switching time in a TB chain with a single impurity [18].

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