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Efficient linear scaling method for computing the Landauer-Büttiker conductance

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Abstract. We report on a novel order N algorithm, that allows efficient computation of the Landauer-Büttiker conductance formula in heterojunctions of any complexity. The method is based on the recursive construction of a bi-orthogonal basis, in which non-hermitian hamiltonian matrices are first tridiagonalized, and continued-fraction expansion further used to accurately compute off-diagonal Green's function matrix elements. The method, of broad range of applicability, is here validated on tight-binding hamiltonians for nanotube-based intramolecular junctions.

PACS. 73.63.Fg Nanotubes – 71.15.-m Methods of electronic structure calculations – 73.63.-b Electronic transport in nanoscale materials and structures – 73.22.-f Electronic structure of nanoscale materials: clusters, nanoparticles, nanotubes, and nanocrystals

Today's research efforts in molecular electronics [1] or nanoelectronics rely on both : top-down and bottom-up technologies to synthesize functional molecular based devices and circuits (for instance see [2]), as well as advanced computational schemes that enable low cost predictive studies of operating modes of envisioned devices. Numerical simulation of nanodevices is mainly divided into two parallel research focuses. First, first principles methods are steadily improved to tackle the physico-chemical complexity at the atomistic scale [3], although both large scale simulations and out-of equilibrium problems are of limited implementation. On the other hand, semi-empirical approaches enable calculations on large scale systems [4], albeit limited to effective hamiltonians with adjustable parameters. The combination of both approaches opens new perspectives to circumvent intrinsic limitations of the separated methods. To envision assessment of large scale device operating modes, it is essential to develop efficient order N methods for the computation of current-voltage characteristics (or similarly conductance spectra).

Efficient computational recursion and order N methods have been widely employed in solid-state physics since their introduction by Haydock [5–7]. The recursion method is based on an eigenvalue approach of Lanczos [8], and is a completely real-space procedure based on Green's functions. This technique is thus particularly well suited for treating disorder and defect-related problems, and has been successfully implemented to tackle impurity-level calculations in semiconductors using the tight-binding approximation[9], and electronic structure investigations for amorphous semiconductors, transition metals and metallic glasses based on linear-muffin-tin orbitals [10]. Initially, it was extensively employed for computing density of states, although electronic conductivities, within the Kubo formalism [11], have also been investigated for disordered metals [12], or even extended recently to treat intrinsic conduction mechanism in nanoscopic systems such as carbon nanotubes [13]. Notwithstanding, to date, no similar efficient algorithm has been implemented for the calculation of Landauer-Büttiker conductance [14,15], given that the general problem involves non-hermitian matrices for which the conventional Lanczos technique fails to construct a tridiagonal basis.

In this work, an efficient algorithm is proposed to extend the functionality of recursion-like methods to quantum transport in heterojunctions. It is based on the construction of a bi-orthogonal basis that is able to tridiagonalize the non-hermitian effective hamiltonian of the system coupled to electrodes, enabling accurate and numerically stable computation of off-diagonal Green's function coefficients through the continued-fraction expansion. Such an approach offers new perspectives for *very large scale computation of quantum transport in molecular devices.*

The general electronic transport theory in the linear response regime relies on the approach derived by R. Kubo [11]. In its zero frequency limit, it reduces to the trace of the operator $\delta(E-H)\hat{V}_x\delta(E-H)\hat{V}_x$, that relates the spectral measure operator $\delta(E-H)$ to the velocity

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operator $\hat{V}_x$. Electronic dc-conductivity is thus seen as a measure of autocorrelation average of wavepackets velocities. Landauer and Büttiker have generalized the transport theory for heterojunctions in terms of a transmission method [14], an approach that has also been reformulated in rewritting the conductance as a trace of a given operator (for instance see [15]). Such a formula has the advantage of being general, independent of the dimensionality of the system and its eventual geometrical and physicochemical complications. To express an analytical form for the conductance of the system under study, it is convenient to dissociate it from the two metallic external electrodes that serve to inject current in and out of the system. This allows us to assume a suitably well-defined form for incoming and outgoing scattering states. These electrodes are further connected to measurement reservoirs, in which energy dissipation finally takes place. Without loss of generality, in the coherent regime the trace formula for the conductance at energy E reads:

$$\mathcal{G}(E) = \frac{2e^2}{h}\mathrm{Tr}\Big[\mathit{\Gamma}_L(E)G^r(E)\mathit{\Gamma}_R(E)G^a(E)\Big]. \qquad (1)$$

The $\mathit{\Gamma}_{L,R}(E) = i[\mathit{\Sigma}^r_{L,R}(E) - \mathit{\Sigma}^a_{L,R}(E)]$ are operators related to the so-called self-energy operators $\mathit{\Sigma}^{r,a}_{L,R}(E)$ containing all the information concerning coupling between the system and the left (L) and right (R) electrodes. The self-energy can be written as $\mathit{\Sigma}^{r,a}_{L,R}(E) = V^\dagger_{L,R-Sys}g^{r,a}_{L,R}(E)V_{L,R-Sys}$, where V_{L-Sys} (resp. V_{R-Sys}) describes the coupling between the System and the L-electrode (resp. R-electrode), while $g^{r,a}_{L,R}(E)$ are the retarded and advanced surface Green's functions of the electrodes [15]. From these definitions, the Green's function that propagates electronic states inside the system, and which is also needed in the trace formula (1), can be expressed as:

$$G^{r,a}(E) = \frac{1}{E - \mathcal{H}_{Sys} - (\mathit{\Sigma}^{r,a}_L(E) + \mathit{\Sigma}^{r,a}_R(E))} \qquad (2)$$

where $\mathcal{H}_{Sys}$ is the hamiltonian of the system under study, disconnected from the electrodes. To allow numerical calculations of these expressions, the hamiltonian of the system and electrodes must be expressed in terms of a tight-binding expression expanded within an orthonormal basis of orbitals. A simple interface geometry is depicted on Figure 1, but the following development is valid for any complex interface. The matrice V_{R-Sys} couples a finite number N of orbitals α of the system to a finite number of orbitals of the L-electrode. Similarly, V_{L-Sys} couples N' orbitals α' to the R-electrode. N and N' are related to the section of the system close to the interfaces, and to the cut-off distance in the orbital coupling, generally restricted to the first neighbours. The finite range of $V_{L,R-Sys}$ implies the same finite range for the matrices $\mathit{\Gamma}_{L,R}$: $\mathit{\Gamma}_L$ (resp. $\mathit{\Gamma}_R$) only couples together the N (N') orbitals of the system close to the L-electrode (R-electrode). The trace formula (1) can be rewritten as:

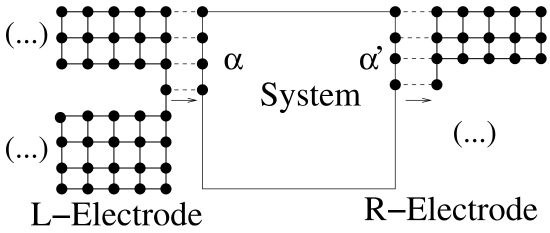

Fig. 1. Simple interface configuration in real space for the heterojunction under consideration. α (resp. α') refer to the localized orbitals of the system coupled to the left (resp. right) electrode.

$$\mathcal{G} = \frac{2e^2}{h}\sum_{\alpha,\beta,\alpha',\beta'}\langle\beta|\mathit{\Gamma}_R|\alpha\rangle\langle\alpha|G^r|\alpha'\rangle\langle\alpha'|\mathit{\Gamma}_L|\beta'\rangle\langle\beta'|G^a|\beta\rangle. \qquad (3)$$

Hereafter, to simplify the notation, the energy dependence is omitted. The interface localized states α, β run over the N orbitals coupled to the L-electrode, and α', β' run over the N' orbitals coupled to the R-electrode. The quantities to calculate are the self-energies $\mathit{\Sigma}^{r,a}_{L,R}$ (which give the $\mathit{\Gamma}_{L,R}$) and the retarded Green's function matrix elements $\langle\alpha|G^r|\alpha'\rangle$. $\mathit{\Sigma}^{r,a}_{L,R}$ are related to the surface Green functions of the semi-infinite electrodes, which are easily computed by standard recursion or decimation techniques. The main task is to evaluate the retarded Green functions $\langle\alpha|G^r|\alpha'\rangle$ which propagate an electron from the right side to the left side of the system. One has to compute $N \times N'$ such matrix elements. The advanced Green's function matrix elements, also needed in equation (3), can then be deduced from the relation $\langle\beta'|G^a|\beta\rangle = (\langle\beta|G^r|\beta'\rangle)^*$.

For calculating each non-diagonal Green's function $\langle\alpha|G^r|\alpha'\rangle$, we first express it as a sum of three diagonal Green's functions as follows

$$\frac{1}{2}\left[(1+i)\langle\psi_+|G^r|\psi_+\rangle + (i-1)\langle\psi_-|G^r|\psi_-\rangle - 2i\langle\psi_i|G^r|\psi_i\rangle\right] \qquad (4)$$

where $|\psi_+\rangle = (|\alpha\rangle + |\alpha'\rangle)/\sqrt{2}$, $|\psi_-\rangle = (|\alpha\rangle - |\alpha'\rangle)/\sqrt{2}$, and $|\psi_i\rangle = (|\alpha\rangle + i|\alpha'\rangle)/\sqrt{2}$.

The problem is thus reduced to the evaluation of $\langle\psi|G^r|\psi\rangle$, where $|\psi\rangle$ is a normalized state. To be used in this context, the recursion approach must be generalized to the case of *non-hermitian matrices*. Indeed, equation (2) contains an effective non-hermitian hamiltonian $\mathcal{H} = \mathcal{H}_{Sys} + \mathit{\Sigma}^r_L + \mathit{\Sigma}^r_R$ describing the finite system coupled to the electrodes. A generalization of the recursion method to the computation of electronic spectra of non-symmetric hamiltonians was tentatively proposed[16], but its further implementation has received little consideration until the work of Benoit et al., who applied a similar approach in a totally different context [17]. As demonstrated below, it can actually be efficiently implemented to the Landauer-Büttiker formalism, which yields a stable, efficient novel computing tool for nanoelectronics.

Starting from the normalized vector $|\psi\rangle$ and from the non-hermitian matrix $\mathcal{H}$, we construct a bi-orthogonal basis $\{|\psi_n\rangle, \langle\phi_n|\}$ defined as follows

$$|\psi_{n+1}\rangle = \mathcal{H}|\psi_n\rangle - a_{n+1}|\psi_n\rangle - b_n|\psi_{n-1}\rangle \qquad (5)$$

$$\langle\phi_{n+1}| = \langle\phi_n|\mathcal{H} - \langle\phi_n|a_{n+1} - \langle\phi_{n-1}|b_n \qquad (6)$$

with the initial conditions $|\psi_{-1}\rangle = |\phi_{-1}\rangle = 0$, $|\psi_0\rangle = |\phi_0\rangle = |\psi\rangle$, and the bi-orthogonality condition

$$\langle\phi_n|\psi_m\rangle = 0 \text{ if } n \neq m. \qquad (7)$$

This last condition is equivalent to the following relations for a_n and b_n:

$$a_n = \frac{\langle\phi_n|\mathcal{H}|\psi_n\rangle}{\langle\phi_n|\psi_n\rangle} \qquad (8)$$

$$b_n = \frac{\langle\phi_{n-1}|\mathcal{H}|\psi_n\rangle}{\langle\phi_{n-1}|\psi_{n-1}\rangle} = \frac{\langle\phi_n|\psi_n\rangle}{\langle\phi_{n-1}|\psi_{n-1}\rangle}. \qquad (9)$$

The four equations (5), (6), (8), and (9) allow recursive determination of the bi-orthogonal basis and of the coefficients a_n, b_n. Note that in "ket" notation, equation (6) must be understood as: $|\phi_{n+1}\rangle = \mathcal{H}^\dagger|\phi_n\rangle - a^*_{n+1}|\phi_n\rangle - b^*_n|\phi_{n-1}\rangle$. One starts from $|\phi_0\rangle = |\psi_0\rangle = |\psi\rangle$. At step 0, one computes $\mathcal{H}|\psi_0\rangle$ and $a_1 = \langle\phi_0|\mathcal{H}|\psi_0\rangle/\langle\phi_0|\psi_0\rangle$ by expanding all the amplitudes within the tight-binding localized basis. $|\psi_1\rangle$ and $|\phi_1\rangle$ are then obtained by computing $\mathcal{H}|\psi_0\rangle - a_1|\psi_0\rangle$ and $\mathcal{H}^\dagger|\phi_0\rangle - a_1^*|\phi_0\rangle$, while the first coefficient b_1 is subsequently deduced from equation (9). At step 1, $\mathcal{H}|\psi_1\rangle$ is computed together with $a_2 = \langle\phi_1|\hat{\mathcal{H}}|\psi_1\rangle/\langle\phi_1|\psi_1\rangle$. Then $|\psi_2\rangle$ and $|\phi_2\rangle$ result from the computation of vectors $\mathcal{H}|\psi_1\rangle - a_2|\psi_1\rangle - b_1|\psi_0\rangle$ and $\mathcal{H}^\dagger|\phi_1\rangle - a_2^*|\phi_1\rangle - b_1^*|\phi_0\rangle$. Finally, the coefficient b_2 is then deduced from equation (9). Steps $n \geq 2$ are exactly similar to step 1. In the basis $\{|\psi_n\rangle\}$, $\mathcal{H}$ has thus a tridiagonal form:

$$H = \begin{pmatrix} a_1 & b_1 & & & \\ 1 & a_2 & b_2 & & \\ & 1 & a_3 & b_3 & \\ & & 1 & . & . \\ & & & . & . \end{pmatrix}. \qquad (10)$$

Hence the recurrence relations (5) and (6) lead to a non-symmetric matrix and to a non-normalized bi-orthogonal basis. By choosing a different convention, a symmetric tridiagonal matrix and/or a normalized basis could be obtained. But the present convention gives better numerical stability in the examples considered hereafter.

The quantity $\langle\psi|G^r(z = E \pm 0^+)|\psi\rangle = \langle\phi_0|\frac{1}{z-\mathcal{H}}|\psi_0\rangle$ can then be computed by the continued fraction method. It is equal to the first diagonal element of $(z-H)^{-1}$ where H is the tridiagonal matrix (10). Let us call $G_0(z)$ this matrix element and define $G_n(z)$, the first diagonal element of the matrix $(z-H_n)^{-1}$, with H_n the matrix H without its n first lines and columns:

$$H_n = \begin{pmatrix} a_n & b_n & & & \\ 1 & a_{n+1} & b_{n+1} & & \\ & 1 & a_{n+2} & b_{n+2} & \\ & & 1 & . & . \\ & & & . & . \end{pmatrix}. \qquad (11)$$

From standard linear algebra, it can be shown that

$$G_0(z) = \frac{1}{z - a_1 - b_1 G_1(z)}, \qquad (12)$$

and replicating such an algorithm, one obtains a continued-fraction of $G_0(z)$:

$$G_0(z) = \cfrac{1}{z - a_1 - \cfrac{b_1}{z - a_2 - \cfrac{b_2}{\cdots}}}. \qquad (13)$$

In contrast with the standard recursion method, the recursion coefficients a_n and b_n do not show any simple behaviour for large n. In the type of applications considered here, a simple truncation of the continuous fraction at sufficiently large n gave a good convergence. One notes that for large systems, recursion coefficients computed by the bi-orthogonal process might experience significant fluctuations, so that a suitable renormalization procedure could be necessary to control convergence of the algorithm [17–19].

To summarize, the evaluation of the diagonal Green's functions $\langle\psi|G^r(z)|\psi\rangle$ is done by a bi-orthogonal recursion approach and a continued fraction expansion. This allows the computation of off-diagonal Green's functions via equation (4). The calculation of the Landauer-conductance is then straightforwardly achieved from equation (3). Note that the diagonal Green's function calculated by this generalized recursion method can also give the local density of states on chosen orbitals of the system coupled to the electrodes.

Let us discuss the numerical cost of this algorithm. With this generalized recursion method, the computation of a single off-diagonal Green's function element $\langle\alpha|G^r|\alpha'\rangle$ requires a number of operations which scales linearly with the number $\mathcal{N}$ of orbitals in the system, as for the standard recursion method. This single fact makes this algorithm very promising for systems which have large transverse dimensions at least in some parts. Indeed, the well-known decimation or transfer matrix techniques are unable to treat systems with too large transverse dimensions, since they require matrix inversion of a layer hamiltonian [25]. Here, in the less favourable case, the number of Green's function elements to calculate is $N \times N'$ (defined above). If we consider for instance a cylinder of width W and length L, N and N' are proportional to W^2 and $\mathcal{N}$ is proportional to $L \times W^2$. The numerical cost is then proportional to $L \times W^6$, similar to standard decimation or transfer matrix techniques [25]. Fortunately, the number of incoming and outgoing modes in the electrodes are often much smaller

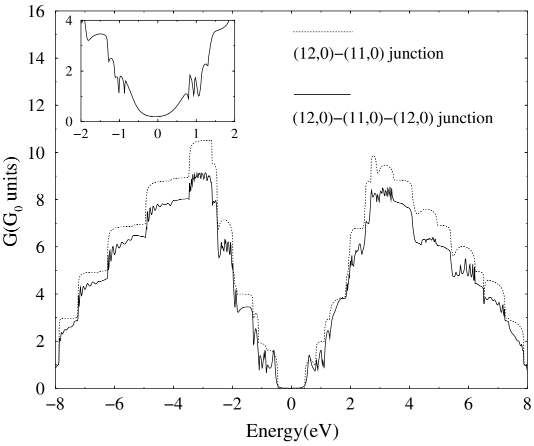

Fig. 2. Electronic conductances of several nanotube-based heterojunctions. Main frame: Simple junction compared with double junction (12,0)-(11,0)-(12,0) junction with length of (11,0) in order of 5 nm. Inset: double junction with length of (11,0) smaller than 3 nm.

than N and N'. The number of Green's function elements to calculate is thus much reduced, and the numerical cost is essentially proportional to $\mathcal{N}$, whatever the geometry and topological complexity of the system.

As an illustration, the Landauer-Büttiker conductance of several nanotube based junctions are computed. The central part is a finite nanotube, which is connected to two semi-infinite tubes with the same or different helicities. We here concentrate on junctions of nanotubes with different helicities. Such intramolecular junctions can be made owing to the introduction of topological disorder such as pentagon-heptagon pair defects. Their theoretical study was pioneered by Ph. Lambin et al. [23] and Chico et al. [20], and is presently the subject of many studies [20–22]. Recently, experimental evidence of such junctions was reported [24] thanks to accurate atomic-scale STM studies. We here concentrate on the (11,0)-(12,0) junction between a metallic and a semiconducting tube.

The results obtained are in full agreement with prior studies [23,20], with in particular a conductance gap driven by the semiconducting tube, and a slight damping of conductance of the junction with respect to the perfect single tube devices. Calculations have also been performed with a more standard procedure [25] and give identical results. The case of the double-junction deserves particular attention given its relevance to molecular electronics. Indeed, such a metal/semiconductor/metal junction can provide important information about the design of molecular quantum dot or spin devices [26]. In Figure 2, the conductance is given for a central part of the device made by the semiconducting tube $(11,0)$ with length 100nm, while external leads are provided by semi-infinite (12,0) metallic tubes. First, one notes that whenever the length of the $(11,0)$-tube is less than 3nm, then direct tunneling between evanescent scattering states of external leads occurs within the gap of the system. These states correspond to the *metal-induced gap states* (MIGS) of bulk the metal/semiconducting interface, and will play a crucial role in the Schottky barrier features of the devices [27]. In contrast, as soon as the tube length becomes larger than 3 nm, direct tunneling is suppressed within the $(11,0)$-gap, which can then begin to really act as a switching canal in a field-effect transistor device.

In conclusion, we have proposed a novel scheme for implementing an order N approach to the calculation of Landauer-Büttiker conductance, a formula that gives direct access to current-voltage responses in the coherent transport regime, and can be straightfowardly generalized to out-of-equilibrium situations [15]. The numerical cost is moderate, roughly scaling with the number of orbitals of the studied system, and by avoiding any diagonalization steps, it potentially outperforms any alternative recursive and decimation-based approaches. Illustration to the case of carbon-nanotubes based intramolecular junctions was reported as a demonstration of computational capability, here limited to the application of effective tight-binding hamiltonian. Its extension to order N ab-initio real space methods deserves further consideration.

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