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Electronic transport in extended systems: Application to carbon nanotubes

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We present an efficient approach to describe the electronic transport properties of extended systems. The method is based on the surface Green's function matching formalism and combines the iterative calculation of transfer matrices with the Landauer formula for the coherent conductance. The scheme is applicable to any general Hamiltonian that can be described within a localized orbital basis. As illustrative examples, we calculate transport properties for various ideal and mechanically deformed carbon nanotubes using realistic orthogonal and nonorthogonal tight-binding models. In particular, we observe that bent carbon nanotubes maintain their basic electrical properties even in the presence of large mechanical deformations.
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I. INTRODUCTION

Recent years have witnessed a great amount of research in the field of quantum conductance in nanostructures.[1] These have become the systems of choice for investigations of electrical conduction on a mesoscopic scale. The improvements in nanostructured material production have stimulated developments in both experiment and theory. In particular, the formal relation between conduction and transmission, the Landauer formula,[2] has enhanced the understanding of electronic transport in extended systems and has proven to be very useful in interpreting experiments involving the conductance of nanostructures. Among all the possible nanostructure materials, carbon nanotubes have attracted much attention since their discovery in 1991,[3] because of their special geometrical and electronic properties. Their electronic and transmission properties have been studied both experimentally[4–8] and theoretically.[9–13] In particular, from the theoretical point of view, the sensitivity of their electronic properties to their geometry makes them truly unique in offering the possibility of studying quantum transport in a very tunable environment.

The problem of calculating quantum conductance in carbon nanotubes has been addressed with a variety of techniques that reflect the various approaches in the theory of quantum transport in ballistic systems. Tian and Datta[9] predicted an Aharonov-Bohm-type effect in graphitic tubules in an axial magnetic field combining the Landauer formula with a semiclassical treatment of the transmission probability. Saito *et al.*[10] studied the tunneling conductance of connected carbon nanotubes via the direct calculation of the current density. Chico *et al.*[11] addressed the problem of quantum conductance in carbon nanotubes with defects, efficiently combining a surface Green's-function approach[14] to describe the interface between different tubes with a scattering matrix-based calculation of the transmission function, thus obtaining the conductance via a multichannel generalization of the Landauer formula. The variation of the conductance with the diameter of the carbon nanotubes has been studied by Tamura and Tsukada.[12] They combined the Landauer formula with the explicit calculation of the scattering matrix and an effective-mass approximation to clarify the physical origin of this scaling law. Most recently, the conductance of carbon nanotube wires in the presence of disorder has been addressed by Anantram and Govindan.[13] They have developed an efficient numerical procedure to compute the electronic transmission using a Green's function formalism.

All the previous calculations derive the electronic structure of the carbon nanotube from a simple π-orbital tight-binding Hamiltonian that describes the bands of the graphitic network of the carbon nanotube via a single nearest-neighbor hopping parameter. Since the electronic properties of carbon nanotubes are basically determined by the sp^2 π orbitals, the model gives a reasonably good qualitative description of their behavior and, given its simplicity, it has become the model of choice in a number of theoretical investigations. However, although qualitatively useful to interpret experimental results, this simple Hamiltonian lacks the accuracy that more sophisticated tight-binding (TB) models or *ab initio* methods are able to provide. In the present paper we present an efficient scheme that is particularly suitable for realistic calculations of electronic transport properties in extended systems. The approach we have designed is inspired by the one outlined in Ref. 11, differing from the latter in the use of the generalized Landauer formula for the transmission function proposed by Meir and Wingreen.[15] This generalization makes the present method extremely flexible and applicable to any system described by a Hamiltonian with a localized orbital basis. The present formulation allows us to also fully consider the complete microscopic structure of the semi-infinite leads (in a lead-conductor-lead geometry) with a very limited computational cost. Moreover, the only quantities that enter into the present formulation are the matrix elements of the Hamiltonian operator, with no need for the explicit knowledge of the electron wave functions for the multichannel expansion. The last fact makes the numerical

FIG. 1. A conductor described by the Hamiltonian H_C, connected to leads L and R, through the coupling matrices h_{LC} and h_{CR}.

calculations particularly efficient also for systems described by multiorbital localized-basis Hamiltonians.

The paper is structured as follows: in Sec. II we introduce the relation between conductance and Green's functions; in Sec. III we introduce the Green's function formalism to compute bulk conductance (III A) and the transmission through an interface (III B). Section IV is devoted to the discussion of the first results obtained with the present method. In particular, we computed the electronic transport in a bent carbon nanotube using a full sp^3 tight-binding Hamiltonian.[16] Our calculations predict that bending does not drastically change the conductivity of the system, and that carbon nanotubes maintain their electric properties even under severe deformations in the absence of topological defects. As an application to the nonorthogonal orbital basis case, we compute the electronic and transport properties of various nanotubes using a nonorthogonal tight-binding scheme[17] based on *ab initio* density-functional theory. We conclude with some final remarks in Sec. V. The appendixes are devoted to the extension of the present method to the general case of a system described by a nonorthogonal Hamiltonian model (Appendix A) and to a truly three-dimensional system (Appendix B).

II. ELECTRON TRANSMISSION AND GREEN'S FUNCTIONS

Let us consider a system composed of a conductor C connected to two semi-infinite leads, R and L, as in Fig. 1. A

fundamental result in the theory of electronic transport is that the conductance through a region of interacting electrons (the C region in Fig. 1) is related to the scattering properties of the region itself via the Landauer formula:[2]

$$\mathcal{C} = \frac{2e^2}{h}\mathcal{T},$$

where $\mathcal{T}$ is the transmission function and $\mathcal{C}$ is the conductance. The former represents the probability that an electron injected at one end of the conductor will transmit to the other end. The transmission function can be expressed in terms of the Green's functions of the conductors and the coupling of the conductor to the leads:[18,19,15]

$$\mathcal{T} = \mathrm{Tr}(\Gamma_L G_C^r \Gamma_R G_C^a),$$

where $G_C^{\{r,a\}}$ are the retarded and advanced Green's functions of the conductor, and $\Gamma_{\{L,R\}}$ are functions that describe the coupling of the conductor to the leads. To compute the Green's function of the conductor we start from the equation for the Green's function of the whole system:

$$(\epsilon - H)G = I, \tag{1}$$

where $\epsilon = E + i\eta$ with η arbitrarily small and I is the identity matrix. In the hypothesis that the Hamiltonian of the system can be expressed in a discrete real-space matrix representation, the previous equation corresponds to the inversion of an infinite matrix for the open system, consisting of the conductor and the semi-infinite leads. The above Green's function can be partitioned into submatrices that correspond to the individual subsystems,

$$\begin{pmatrix} G_L & G_{LC} & G_{LCR} \\ G_{CL} & G_C & G_{CR} \\ G_{LRC} & G_{RC} & G_R \end{pmatrix} = \begin{pmatrix} (\epsilon - H_L) & h_{LC} & 0 \\ h_{LC}^\dagger & (\epsilon - H_C) & h_{CR} \\ 0 & h_{CR}^\dagger & (\epsilon - H_R) \end{pmatrix}^{-1}, \tag{2}$$

where the matrix $(\epsilon - H_C)$ represents the finite isolated conductor, $(\epsilon - H_{\{R,L\}})$ represent the infinite leads, and h_{CR} and h_{LC} are the coupling matrices that will be nonzero only for adjacent points in the conductor and the leads, respectively. From this equation it is straightforward to obtain an explicit expression for G_C:[18]

$$G_C = (\epsilon - H_C - \Sigma_L - \Sigma_R)^{-1}, \tag{3}$$

where we define $\Sigma_L = h_{LC}^\dagger g_L h_{LC}$ and $\Sigma_R = h_{RC} g_R h_{RC}^\dagger$ as the self-energy terms due to the semi-infinite leads and $g_{\{L,R\}} = (\epsilon - H_{\{L,R\}})^{-1}$ are the leads' Green's functions. The self-energy terms can be viewed as effective Hamiltonians that arise from the coupling of the conductor with the leads. Once the Green's functions are known, the coupling functions $\Gamma_{\{L,R\}}$ can be easily obtained as[18]

$$\Gamma_{\{L,R\}} = i[\Sigma_{\{L,R\}}^r - \Sigma_{\{L,R\}}^a],$$

where the advanced self-energy $\Sigma_{\{L,R\}}^a$ is the Hermitian conjugate of the retarded self-energy $\Sigma_{\{L,R\}}^r$. The core of the problem lies in the calculation of the Green's functions of the semi-infinite leads. In what follows we will present an efficient approach to compute the self-energy terms in the general case of an arbitrary localized-orbital Hamiltonian.

III. GREEN'S FUNCTIONS AND CONDUCTIVITY FROM THE LAYER HAMILTONIAN

A. Transmission through a bulk system

It is well known that any solid (or surface) can be viewed as an infinite (semi-infinite in the case of surfaces) stack of

principal layers with nearest-neighbor interactions.[20] This corresponds to transforming the original system into a linear chain of principal layers. Within this approach, the matrix elements of Eq. (1) between layer orbitals will yield a set of equations for the Green's functions:

$$(\epsilon - H_{00})G_{00} = I + H_{01}G_{10},$$

$$(\epsilon - H_{00})G_{10} = H_{01}^{\dagger}G_{00} + H_{01}G_{20},$$

$$\ldots, \tag{4}$$

$$(\epsilon - H_{00})G_{n0} = H_{01}^{\dagger}G_{n-1,0} + H_{01}G_{n+1,0},$$

where H_{nm} and G_{nm} are the matrix elements of the Hamiltonian and the Green's function between the layer orbitals, and we assume that in a bulk system $H_{00} = H_{11} = \ldots$ and $H_{01} = H_{12} = \ldots$. Following Lopez-Sancho et al.,[21] this chain can be transformed in order to express the Green's function of an individual layer in terms of the Green's function of the preceding (or following) one. This is done via the introduction of the transfer matrices T and $\bar{T}$, defined such that $G_{10} = TG_{00}$ and $G_{00} = \bar{T}G_{10}$. The transfer matrix can be easily computed from the Hamiltonian matrix elements via an iterative procedure, as outlined in Ref. 21. In particular T and $\bar{T}$ can be written as

$$T = t_0 + \tilde{t}_0 t_1 + \tilde{t}_0 \tilde{t}_1 t_2 + \ldots + \tilde{t}_0 \tilde{t}_1 \tilde{t}_2 \cdots t_n,$$

$$\bar{T} = \tilde{t}_0 + t_0 \tilde{t}_1 + t_0 t_1 \tilde{t}_2 + \ldots + t_0 t_1 t_2 \cdots \tilde{t}_n,$$

where t_i and $\tilde{t}_i$ are defined via the recursion formulas:

$$t_i = (I - t_{i-1}\tilde{t}_{i-1} - \tilde{t}_{i-1}t_{i-1})^{-1}t_{i-1}^2,$$

$$\tilde{t}_i = (I - t_{i-1}\tilde{t}_{i-1} - \tilde{t}_{i-1}t_{i-1})^{-1}\tilde{t}_{i-1}^2$$

and

$$t_0 = (\epsilon - H_{00})^{-1}H_{01}^{\dagger},$$

$$\tilde{t}_0 = (\epsilon - H_{00})^{-1}H_{01}.$$

The process is repeated until $t_n, \tilde{t}_n \leq \delta$ with δ arbitrarily small.[22]

With this proviso, we can write the bulk Green's function as

$$G(E) = (\epsilon - H_{00} - H_{01}T - H_{01}^{\dagger}\bar{T})^{-1}.$$

If we compare the previous expression with Eq. (2) in the hypothesis of leads and conductors being of the same material (bulk conductivity),[23] we can identify the present bulk system, or rather one of its principal layers, with the conductor C, so that $H_{00} \equiv H_C$, $H_{01} \equiv h_{CR}$, and $H_{01}^{\dagger} \equiv h_{LC}^{\dagger}$. In particular, by comparing with Eq. (3), we obtain the expression of the self-energies of the conductor-leads system:

$$\Sigma_L = H_{01}^{\dagger}\bar{T}, \quad \Sigma_R = H_{01}T.$$

The coupling functions are then obtained from the sole knowledge of the transfer matrices and the coupling Hamil-
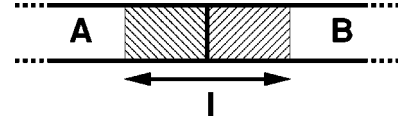
tonian matrix elements: $\Gamma_L = -\mathrm{Im}(H_{01}^{\dagger}\bar{T})$ and $\Gamma_R = -\mathrm{Im}(H_{01}\bar{T})$. $N.B.$ The knowledge of the bulk Green's function G gives also direct informations on the electronic spectrum via the spectral density of bulk electronic states: $N(E) = -(1/\pi)\mathrm{Im}[\mathrm{Tr}G(E)]$.

FIG. 2. Sketch of a system containing an interface. I is the interface region for which we need to compute the Green's function G_I.

B. Transmission through an interface

The procedure outlined above can also be applied in the case where electron transmission takes place through an interface between two different media, as in the system depicted in Fig. 2. To study this case we make use of the surface Green's function matching (SGFM) theory, pioneered by Garcia-Moliner and Velasco.[14]

We have to solve Eq. 1 for $H = H_I$ and $G = G_I$, where the subscript I refers to the interface region. Using the SGFM method, G_I is calculated from the bulk Green's function of the isolated systems G_A and G_B, and the coupling between the two sides of the interface, H_{AB} and H_{BA}. In the language of Ref. 14, all these quantities can be expressed using 2×2 supermatrices, defined via the introduction of the appropriate projection operators that map the subspaces of the different materials. In particular we can define $P = P_A + P_B$ where P is the projector in the space of the existing orbitals, and $I_I = I_A + I_B$ is the projector of the interface region. The bulk Hamiltonian $H_{\{A,B\}}$ is meaningful only if related with the corresponding part of P and I_I. For example, the interface part of the bulk Green's function for material A is given by

$$\mathcal{G}_A = I_A G_A I_A = \begin{pmatrix} G_A & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathcal{G}_A^{-1} = \begin{pmatrix} G_A^{-1} & 0 \\ 0 & 0 \end{pmatrix},$$

and $\mathcal{G}_A^{-1}\mathcal{G}_A = I_A$.

Let us now consider the propagation of an elementary electronic excitation in the system. Via the calculation of the transmitted and reflected amplitudes of an excitation that propagates from medium A to medium B, it can be shown that the interface Green's function obeys the following secular equation:[14]

$$G_I^{-1} = (I_A \epsilon I_A - I_A H_A P_A G_A \mathcal{G}_A^{-1}I_A) + (I_B \epsilon I_B$$
$$- I_B H_B P_B G_B \mathcal{G}_B^{-1}I_B) - (I_A H_I I_B + I_B H_I I_A).$$

In the language of layer Hamiltonians and block supermatrices, the previous equation reads
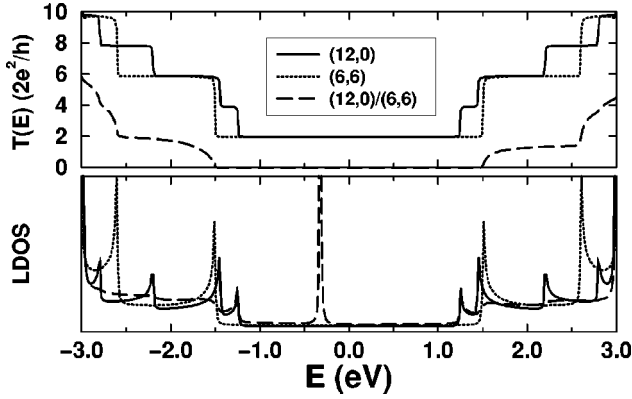
FIG. 3. LDOS and transmission function for the $(12,0)/(6,6)$ matched tube as in Chico *et al.* (Ref. 11). The peak in the LDOS just below the Fermi energy (taken as reference) was not shown in Fig. 4 of Ref. 11 due to a coarser sampling of the energy (see Ref. 31). Besides this, the two calculations are in complete agreement.

$$G_I = \begin{pmatrix} G_{AA} & G_{AB} \\ G_{BA} & G_{BB} \end{pmatrix}$$

$$= \begin{pmatrix} \epsilon - H_{00}^A - (H_{01}^A)^\dagger \bar{T} & -H_{AB} \\ -H_{BA} & \epsilon - H_{00}^B - H_{01}^B T \end{pmatrix}^{-1} . \quad (5)$$

Once the interface Green's function is known, we can compute the transmission function in terms of block supermatrices making use of the interface projection operators:

$$\mathcal{T}(E) = \mathrm{Tr}(\Gamma_L G_I^r \Gamma_R G_I^a), \quad \Gamma_L = I_A \Gamma_A I_A, \quad \Gamma_R = I_B \Gamma_B I_B .$$

Using Eq. (5) we can write, after some matrix multiplications:

$$\mathcal{T}(E) = \mathrm{Tr}(\Gamma_A G_{AB}^r \Gamma_B G_{BA}^a)$$

and $G_{BA}^a = (G_{AB}^r)^\dagger$. Within the SGFM framework, the same approach can be extended to the case of multiple interfaces, superlattices, and the general lead-conductor-lead geometry[14] with little complication. In the previous treatment we have assumed to have a Hamiltonian representation in terms of orthogonal orbitals. The extension to the general case of a nonorthogonal base is described in Appendix A. We have also assumed a truly one-dimensional chain of principal layers, which is physical only for systems like nanotubes or quantum wires that have a definite quasi-one-dimensional character. The straightforward extension to a truly three-dimensional case is described in Appendix B. *N.B.* As in the bulk case, we can calculate the local density of states localized at the interface as $N_I(E) = -(1/\pi)\mathrm{Im}[\mathrm{Tr}G_I(E)]$.

IV. EXAMPLES

As a first application of the above methodology we studied the quantum conductance of carbon nanotubes within a nearest-neighbor π-orbital tight-binding Hamiltonian as in Chico *et al.*[11] In this model, the π-orbital bands are described via a single parameter $V_{pp\pi} = \gamma_0 = -2.75$ eV. As shown in Fig. 3, we were able to completely reproduce the results for the conduction of a $(12,0)/(6,6)$ matched nanotube

obtained in Ref. 11. Although this simple model can give a reasonable qualitative description of the electronic and transport properties of an ideal carbon nanotube, more sophisticated models have to be used for a more general study. In particular, geometric relaxations are ineffective in the π-orbital tight-binding model, where only the connectivity of a given atom plays a role. In order to study the effect of atomic relaxations on the conductance of carbon nanotubes, we employed a full sp^3 tight-binding model already used in the studies of electronic properties of such systems.[16] One of the advantages of the present method to compute quantum conductance is that it does not require periodic boundary conditions along the direction of the principal layer expansion. In quasi-one-dimensional systems such as nanotubes and nanowires, this implies that very distorted geometries can be analyzed with a complete convergence in the (one-dimensional) $k_\perp$-point expansion (see Appendix B).

In the following we present our investigations of the effect that bending has in the transport properties of a small diameter $(4,4)$ carbon nanotube. It has recently been observed[7] that individual carbon nanotubes deposited on a series of electrodes behave as a chain of quantum wires connected in series. The individual nanotube is broken up into a chain of weakly coupled one-dimensional conductors separated by local barriers. It has been argued that the local barriers arise from the bending of the tube near the edge of the electrodes, but no theoretical evidence has been produced as yet. In the upper part of Fig. 4 we show the system that we have studied: an initially straight tube that has been bent at different angles $\theta = 0°, 3°, 6°$ [Figs. 4 (a)–4(c)], where θ measures the inclination of the two ends of the tubes with respect to the unbent axis. The geometrical structure has been optimized using an empirical many-body potential for carbon.[24] For $\theta = 6°$ we observe the formation of a kink. Since the formation of kinks in bent carbon nanotubes has been thoroughly described both experimentally and theoretically,[25] we do not discuss it here. In the lower part of Fig. 4 we present our predictions for electronic conductance and density of states of the bent tube. The presence of the kink does not alter drastically the local density of states (LDOS) at the interface nor the conductance of the system in a substantial manner. This observation rules out the possibility that the formation of local barriers for electric transport can be attributed solely to the microscopic deformation of the tube wall, with no defect involved. The effect of defects that will naturally form in the bent tube due to the strain imposed on the system[26] has not been taken into account, and it will be the subject of future work.[27]

In Fig. 5 we show the LDOS and transmission function for a semiconducting $(10,0)$ and metallic $(9,0)$ nanotubes calculated using an orthogonal and a nonorthogonal TB model. Both models reproduce the general features of the electronic structure, in particular the opening of a pseudogap at the Fermi energy produced by the curvature of the graphitic walls in the $(9,0)$ nanotube.[28,29] The values of the gap calculated with the orthogonal (0.07 eV) and nonorthogonal TB (0.16 eV) are in very good agreement with previous calculations,[28,29] and the nonorthogonal model reproduces quite accurately the *ab initio* value.[29] The extension of the present method to nonorthogonal Hamiltonians opens a way to calculations of conductance using *ab initio* real-space
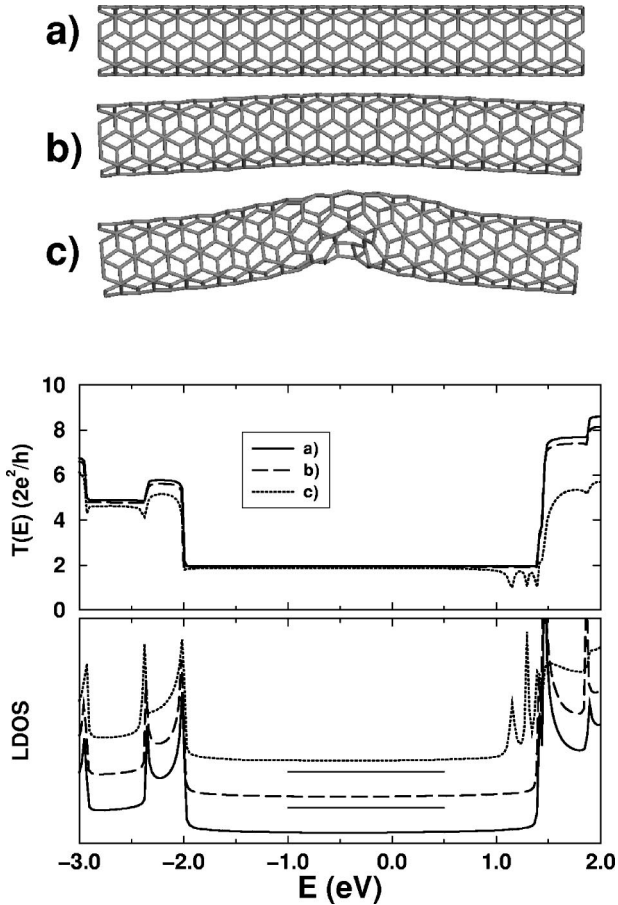
FIG. 4. Upper panel: geometry of the bent (4,4) nanotube used in the calculations. Lower panel: LDOS and transmission function for the different geometries: (a) $\theta=0°$, (b) $3°$, (c) $6°$. LDOS's for different bending angles are shifted in the picture. The Fermi energy is always taken as a reference.

methods with nonorthogonal localized-orbital bases. Work in this direction is in progress and will be the subject of a future publication.[30]

V. CONCLUSIONS

In this paper we presented an efficient approach to compute the electronic transport properties of extended systems and some applications to carbon nanotubes. The essence of the approach relies on the iterative calculation of transfer matrices and Green's functions coupled with the Landauer formula for the coherent conductance. This method is applicable to any general Hamiltonian that can be described within a localized-orbital basis and thus can be used as an efficient and general theoretical scheme for the analysis of the electrical properties of nanostructures. The applicability of the method to general orthogonal and nonorthogonal tight-binding models has been illustrated. In particular, we have obtained a theoretical analysis of quantum conductance in bent carbon nanotubes. Our calculations show that carbon nanotubes maintain their basic electrical characteristics even in the presence of large distortions and mechanical deformations.
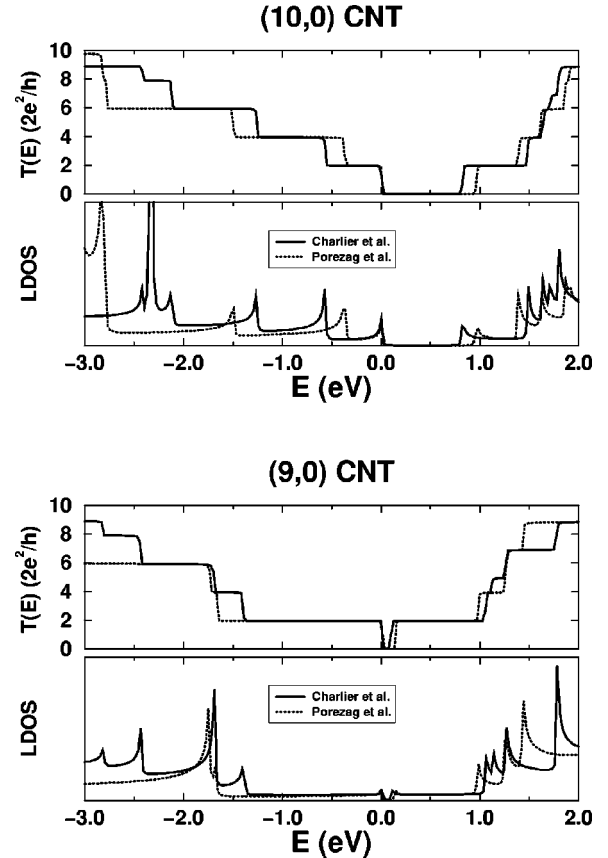

FIG. 5. Upper panel: LDOS and transmission function for a (10,0) carbon nanotube using the nonorthogonal tight-binding of Porezag *et al.* (Ref. 17) compared with the orthogonal model of Charlier *et al.* (Ref. 16) Lower panel: same as above for a (9,0) tube. The Fermi energy is taken as reference.

APPENDIX A

The expression for the Green's and transmission functions of a bulk system described by a general nonorthogonal localized-orbital Hamiltonian follows directly from the procedure outlined in Sec. III A. All the quantities can be obtained making the substitutions: $(\epsilon-H_{00})\rightarrow(\epsilon\mathcal{S}_{00}-H_{00})$ and $H_{01}^{(\dagger)}\rightarrow-(\epsilon\mathcal{S}_{01}^{(\dagger)}-H_{01}^{(\dagger)})$. Here, we introduce the matrices $\mathcal{S}$'s that represent the overlap between the localized orbitals. With this recipe, the equation chain (4) now reads

$$(\epsilon\mathcal{S}_{00}-H_{00})G_{00}=I-(\epsilon\mathcal{S}_{01}-H_{01})G_{10},$$

$$(\epsilon\mathcal{S}_{00}-H_{00})G_{10}=-(\epsilon\mathcal{S}_{01}^{\dagger}-H_{01}^{\dagger})G_{00}$$
$$-(\epsilon\mathcal{S}_{01}-H_{01})G_{20},$$

$$\dots,$$

$$(\epsilon \mathcal{S}_{00} - H_{00})G_{n0} = -(\epsilon \mathcal{S}_{01}^{\dagger} - H_{01}^{\dagger})G_{n-1,0}$$
$$- (\epsilon \mathcal{S}_{01} - H_{01})G_{n+1,0}.$$

From here, via the same series of algebraic manipulations as in the orthogonal case, we obtain the Green's function:

$$G = [(\epsilon \mathcal{S}_{00} - H_{00}) + (\epsilon \mathcal{S}_{01} - H_{01})T + (\epsilon \mathcal{S}_{01}^{\dagger} - H_{01}^{\dagger})\bar{T}]^{-1},$$

and from the latter we can identify the self-energies,

$$\Sigma_L = -(\epsilon \mathcal{S}_{01}^{\dagger} - H_{01}^{\dagger})\bar{T}, \quad \Sigma_R = -(\epsilon \mathcal{S}_{01} - H_{01})T.$$

The extension to the case of the transmission through an interface follows exactly the same lines.

APPENDIX B

The extension of the present scheme to a truly three-dimensional case is very simple. The introduction of the principal layer concept implies that along the direction of the layer expansion the system is described by an infinite set of $k_{\perp}$ while $k_{\parallel}$ is still a good quantum number for the problem. The above procedure effectively reduces the three-dimensional system to a set of noninteracting linear chains, one for each $k_{\parallel}$.[20] We can then use the usual k-point summation techniques to evaluate, for instance, the quantum conductance,

$$T(E) = \sum_{k_{\parallel}} w_{k_{\parallel}} T_{k_{\parallel}}(E),$$

where $w_{k_{\parallel}}$ are the relative weights of the different $k_{\parallel}$'s in the irreducible wedge of the surface Brillouin zone.

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