

# Green's function calculations for semi-infinite carbon nanotubes

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In the modeling of nanoscale electronic devices, the non-equilibrium Green's function technique is gaining increasing popularity. One complication in this method is the need for computation of the "self-energy" functions that account for the interactions between the active portion of a device and its leads. In the one-dimensional case, these functions may be computed analytically. In higher dimensions, a numerical approach is required. In this work, we generalize earlier methods that were developed for tight-binding Hamiltonians, and present results for the case of a carbon nanotube.

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## 1 Introduction

The carbon nanotube field-effect transistor (CNFET) has attracted a great deal of interest due to predictions of its superior performance over that of ultimately scaled silicon MOSFETs [1, 2]. While significant progress has been made in predicting its behaviour, simulations have primarily focused on azimuthally invariant structures, such as the cylindrically-gated CNFET [2, 3]. Although this may be an ideal structure in terms of reducing short-channel effects, it poses serious difficulties in terms of its realization, and as a result, rigorous experimental verification of the theoretical models has proved difficult. In addition, much of the modeling effort has focused on devices with bulk metallic Schottky-barrier contacts [1, 3, 4, 5], while the experimental work with doped nanotube contacts to an intrinsic channel [6, 7] has garnered less theoretical attention [2].

In order to consider doped nanotube contacts, and more experimentally feasible geometries for CNFETs, it is convenient to consider the non-equilibrium Green's function (NEGF) technique [8]. Essentially, we seek the Green's function for a "scattering region" connected to two semi-infinite leads, which in our case are the doped source and drain regions of the nanotube. The Hamiltonian for this system is infinite, but if we are only interested in the scattering region, we may reduce the size of the matrix by computing a self-energy function [8]. In the one-dimensional case, this self-energy has an analytic form [9], and as a result, simplifying assumptions are typically made in order to reduce problems to a single dimension.

For general situations, the self-energy calculations are more complex, and so we present a method for numerically calculating these matrices for systems that are described by an atomistic, tight-binding Hamiltonian. By considering each individual atom, we are able to account for potential variations in the scattering region in more than just the transport direction. In the CNFET case, this method also allows us to consider nanotube chiralities that exhibit less azimuthal symmetry in the atomic positions than the zig-zag case that is typically considered.

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This work extends that of Appelbaum *et al.* [10], where interactions between the scattering region and the leads were described by a scalar quantity, and of Venugopal *et al.* [11], where Hermitian coupling matrices were assumed. In cases where the primitive unit cell has more than a single layer of atoms, the coupling matrices are unlikely to be Hermitian due to the dependence of the coupling matrix elements on distance. This is indeed the case for carbon nanotubes, and hence our generalization is required.

## 2 Methodology

A nearest-neighbour, tight-binding Hamiltonian for an infinitely-long carbon nanotube may be written in the form

$$H = \begin{bmatrix} \ddots & & & & & & \\ & \tau^\dagger & A_L & \tau & & & \\ & & \tau^\dagger & A_S & \tau & & \\ & & & \tau^\dagger & A_R & \tau & \\ & & & & & \ddots & \\ & & & & & & \ddots \end{bmatrix},$$

where we note that a nanotube has periodicity in its atomic positions. Indeed, this method could, in principle, be used for any crystalline material. The periodicity is defined by a primitive unit cell, containing  $n_1$  atoms, which can be translated, with no rotation, in order to tile the entire crystal. Note that the CN unit cell is usually larger than the graphite unit cell due to the requirement of no rotation when translating. Here,  $\tau$  represents the coupling between these primitive unit cells,  $\tau^\dagger$  is the Hermitian conjugate of  $\tau$ ,  $A$  represents both the local potential energy and the coupling between atoms within a primitive unit cell, and the subscripts  $L$ ,  $S$ , and  $R$  represent the left lead, the scattering region, and the right lead, respectively. Note that all of these quantities are matrices, and that the left and right leads extend off to infinity. The magnitude of the atom-atom coupling is given by an overlap integral of atomic wavefunctions, and in the CN case, we take a nominal value of 2.8 eV as appropriate for the  $p_z$  orbitals [12]. In addition, we define the “leads” as regions where the local potential energy becomes constant in the transport direction, so that the rows corresponding to each unit cell of the leads repeat along the diagonal of  $H$  out to infinity. Potential variation normal to the transport direction is permitted in the leads, and any arbitrary potential variation is permitted in the scattering region.

The Green's function, which contains information about the local density of states (LDOS) [8, 9], is given by

$$g = (E - H)^{-1},$$

where  $E$  is energy. Since we are only concerned with the scattering region, we may truncate our infinite matrix using the method described in Ref. [9]. This allows us to compute the Green's function for the scattering region as

$$g_S = (E - A_S - \Sigma_L - \Sigma_R)^{-1},$$

where

$$\Sigma_L = \tau^\dagger g_L \tau, \tag{1}$$

$$\Sigma_R = \tau g_R \tau^\dagger \tag{2}$$

are the self-energies. Note that all of the matrices here are finite, and as a result, the inverse may be computed directly, or by using a recursive algorithm [13]. Note, however, that the recursive

algorithm appears to be numerically unstable, and may result in significant errors being introduced if there are too many layers involved in the recursion. An alternative approach, that results in significant computational savings, is now presented.

Due to the tight-binding form of the Hamiltonian, we can write the self-energies in block form as

$$\Sigma_L = \begin{bmatrix} \sigma_L & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

$$\Sigma_R = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \sigma_R \end{bmatrix},$$

where the diagonal elements, from upper-left to lower-right, have sizes  $n_1 \times n_1$ ,  $(n_S - 2n_1) \times (n_S - 2n_1)$ , and  $n_1 \times n_1$ , respectively, where  $n_S$  is the total number of atoms in the scattering region, and we have assumed, without loss of generality, that  $n_S$  is an integer. The LDOS is given by the diagonal elements [8, 9] of

$$g_S \left( \Sigma_L - \Sigma_L^\dagger + \Sigma_R - \Sigma_R^\dagger \right) g_S^\dagger,$$

and if we write  $g_S$  in block form as

$$g_S = \begin{bmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{bmatrix},$$

we see that the second block column of  $g_S$  is irrelevant. As a result, it is much more computationally efficient to solve

$$(E - A_S - \Sigma_L - \Sigma_R) \begin{bmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{bmatrix} = \begin{bmatrix} I & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & I \end{bmatrix},$$

for  $G_{ij}$ , where  $I$  is the identity matrix. We may, then, compute the LDOS as

$$\text{diag} \left[ G_{i1}(\sigma_L + \sigma_L^\dagger)G_{i1}^\dagger + G_{i3}(\sigma_R + \sigma_R^\dagger)G_{i3}^\dagger \right],$$

where  $i = 1, 2$ , and  $3$  for atoms in the unit cell adjacent to the left lead, away from either lead, and adjacent to the right lead, respectively. It now remains to describe how one may compute  $g_L$  and  $g_R$  in order to obtain the self-energies from Eqs. (1) and (2).

As mentioned previously, Appelbaum *et al.* have presented a method for calculating the required elements of  $g_L$  and  $g_R$  for the case where  $\tau$  is a scalar [10], and Venugopal *et al.* have presented that for the case where  $\tau = \tau^\dagger$  [11]. In our case, we require a generalization of their methods. The Green's function for the left lead,  $g_L$ , is the inverse of

$$E - H_L = \begin{bmatrix} \ddots & & & & \\ \tau^\dagger & E - A_L & \tau & & \\ & \tau^\dagger & E - A_L & \tau & \\ & & \tau^\dagger & E - A_L & \\ & & & & \ddots \end{bmatrix}.$$

Due to the infinite size of this matrix, we can also write this equation compactly as

$$E - H_L = \begin{bmatrix} E - H_L & \tau \\ \tau^\dagger & E - A_L \end{bmatrix}.$$

We define  $g_L$  as

$$g_L = \begin{bmatrix} g_l & g_{ls} \\ g_{sl} & g_s \end{bmatrix} = \begin{bmatrix} E - H_L & \tau \\ \tau^\dagger & E - A_L \end{bmatrix}^{-1}, \quad (3)$$

where  $g_s$  are the surface elements of  $g_L$ .

Eq. (3) may also be written as

$$\begin{bmatrix} E - H_L & \tau \\ \tau^\dagger & E - A_L \end{bmatrix} \begin{bmatrix} g_l & g_{ls} \\ g_{sl} & g_s \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}.$$

We can solve this matrix equation to get

$$g_s = [E - A_L - \tau^\dagger(E - H_L)^{-1}\tau]^{-1}.$$

Of course, this still requires the inversion of an infinite matrix. However, we can, again, exploit the nearest-neighbour, tight-binding structure of  $\tau$  to get that  $\tau^\dagger(E - H_L)^{-1}\tau = \tau^\dagger g_s \tau$ . As a result, our problem now is to solve the nonlinear equation

$$g_s = [E - A_L - \tau^\dagger g_s \tau]^{-1}, \quad (4)$$

which may be most simply done using a fixed-point iterative scheme, as in Ref. [10], such as

$$g_s^{i+1} = [E - A_L - \tau^\dagger g_s^i \tau]^{-1},$$

where the superscript indicates the iteration number.

While this method generalizes that of Refs. [10] and [11], and does appear to converge for all cases attempted thus far, the convergence of the fixed-point method can be quite poor. As a result, we also consider using Newton's method on Eq. (4). We define

$$Q(g_s) = \tau^\dagger g_s \tau g_s - (E - A_L)g_s + I,$$

which is equal to zero when  $g_s$  is the exact solution. This is a quadratic matrix equation, and we seek the error matrix,  $\epsilon$ , that may be applied to some approximate solution,  $\tilde{g}_s$ . We wish to solve

$$Q(\tilde{g}_s + \epsilon) = \tau^\dagger(\tilde{g}_s + \epsilon)\tau(\tilde{g}_s + \epsilon) - (E - A_L)(\tilde{g}_s + \epsilon) + I$$

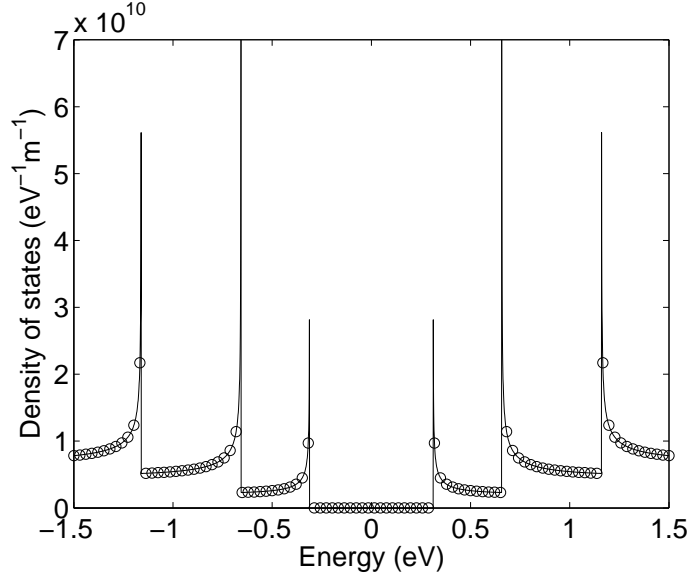
for  $\epsilon$ , where  $Q(\tilde{g}_s) = 0$ . This leads to

$$Q(\tilde{g}_s + \epsilon) = Q(\tilde{g}_s) + D_{\tilde{g}_s}(\epsilon) + \tau^\dagger \epsilon \tau \epsilon,$$

where

$$D_{\tilde{g}_s}(\epsilon) = \tau^\dagger \epsilon \tau \tilde{g}_s + [\tau^\dagger \tilde{g}_s \tau - (E - A_L)]\epsilon \quad (5)$$

is related to the Fréchet derivative of  $Q(\tilde{g}_s)$  in the direction  $\epsilon$ . The Newton method is defined by solving  $Q(\tilde{g}_s) + D_{\tilde{g}_s}(\epsilon) = 0$  for  $\epsilon$ . As noted in Ref. [14], this is a special case of the generalized Sylvester equation, and may be solved using the method described in Ref. [15]. Due to the sensitivity of Newton's method to the initial guess, we damp our iterations using exact line searches



**Fig. 1** Comparison of the standard tight-binding density of states (solid line) with that computed using the self-energy method (circles) for a (16,0) carbon nanotube.

[14], where instead of performing the usual Newton update of  $g_s^{i+1} = g_s^i + \epsilon$ , we use  $g_s^{i+1} = g_s^i + t\epsilon$ , where  $t$  is a parameter chosen such that the square of the Frobenius norm of  $Q(g_s^i + t\epsilon)$  is minimized at each step. Details of this procedure are provided in Ref. [14]. In general, exact line searches were required in order to obtain convergence with Newton's method.

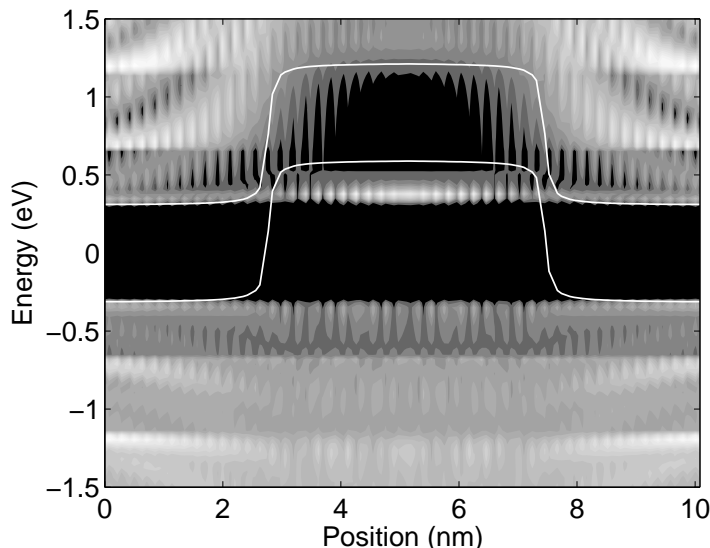
Due to the increased computational effort per iteration for this method, we always begin, in practice, with fixed-point iterations for a while, and then switch to Newton with exact line searches. Typically, only a few Newton iterations are required in this hybrid approach.

A completely analogous procedure holds for the calculation of the surface elements of  $g_R$ , except that we exchange  $\tau$  with  $\tau^\dagger$ , and vice versa, in all of the above derivation.

### 3 Results and Discussion

The simplest case with which we can check our results is for the case where the local potential is some fixed constant. In this case, we have a periodic structure extending out to infinity in both directions, and can, therefore, apply the Bloch condition in order to compute the DOS using a single, primitive CN unit cell. Equivalently, one may employ the “zone-folding scheme” in order to obtain the DOS from the dispersion relation for graphene (see Ref. [16], for example). In our case, we let  $A_L = A_S = A_R$ , and apply our method to compute the DOS from  $g_S$  [8, 9]. In order to numerically handle the van Hove singularities in the CN DOS, energies were perturbed by a small, positive imaginary number. For the results shown here, the perturbation was  $2 \times 10^{-6}i$ , and convergence was declared when the infinity norm of  $Q(\tilde{g}_s)$  became less than  $10^{-6}$ . As shown in Fig. 1, this method produces the correct form.

The second case that we consider is that of a finite barrier. In this case, we expect quantum mechanical reflection for carriers above the barrier, and the possibility of tunneling through the barrier. These phenomena should modify the form of the LDOS at each position. Fig. 2 shows the LDOS for this case, and the solid lines show the conduction and valence band edges shifted by the local potential energy. Regions of high electron concentration are shown as bright patches,



**Fig. 2** Local density of states for a barrier potential in a (16,0) carbon nanotube. Bright patches denote a high density of states, and the solid white lines indicate the conduction and valence band edges shifted by the local potential energy.

and since the Green's function represents outgoing waves at infinity, we obtain a vanishing density in the scattering region for energies lined up with the bandgap in the leads. We also note that the phenomena of interband tunneling, which may have important technological applications [17, 18], is clearly shown in the figure. The jumps in density with energy are due to the contributions of higher bands, and intraband tunneling is also evinced by the penetration of carriers into the bandgap region. We note, here, that in Ref. [8], a subsequent summation was required for each transverse mode, or band, and that these modes were assumed to be independent. In our case, a single calculation provides a complete multiband result with allowed interband transitions.

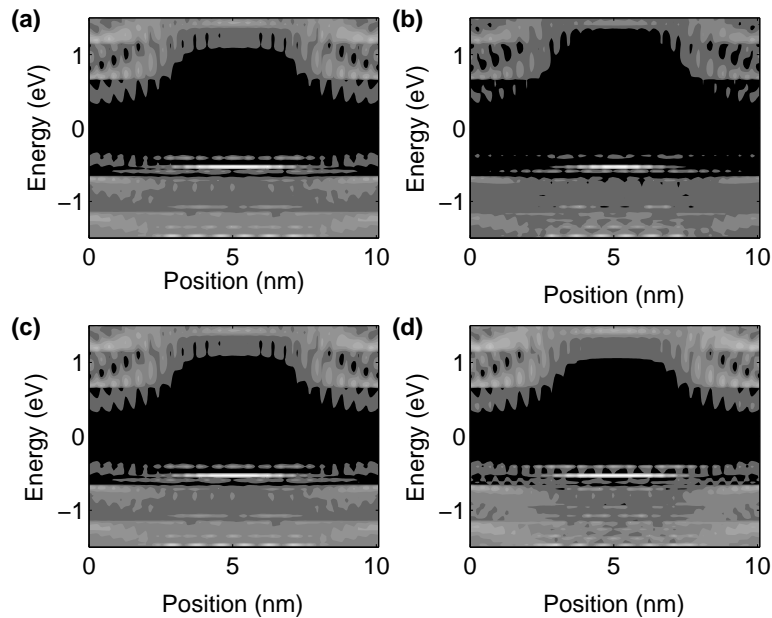
Finally, we compute the LDOS for a potential that varies both azimuthally, and along the length of the CN. A longitudinal potential variation is multiplied by  $1 + 0.1 \sin(\phi)$ , where  $\phi$  is the angular position on the CN surface. Fig. 3 shows the resultant LDOS at  $\phi = 0, \pi/2, \pi$ , and  $3\pi/2$  radians, and the variation with angle is readily identifiable. A one-dimensional approximate solution to this problem would not be able to capture this result.

While this method yields excellent results, further analysis is required due to the possibility of a multiplicity of solutions that may satisfy our quadratic matrix equation. It is well-known that equations of this type may have any number of solutions, including no solution at all. At present, we can only state that there is at least one solution to our equation, and that it is a physically reasonable one.

## 4 Conclusions

From this theoretical work on self-energy calculations for semi-infinite leads connected to a scattering region, it can be concluded that:

1. the methods presented in Refs. [10] and [11] may be generalized to incorporate less restrictive coupling between primitive unit cells of a crystal;



**Fig. 3** Local density of states for both longitudinal and azimuthal potential variation in a (16,0) carbon nanotube at angular positions of (a) 0, (b)  $\pi/2$ , (c)  $\pi$ , and (d)  $3\pi/2$  radians on the nanotube surface.

2. significant computational savings may be realized by only calculating the required elements of the Green's function for the scattering region;
3. calculation of the self-energy functions may be done by solving a quadratic matrix equation using Newton's method, but this is only advisable if exact line searches are employed;
4. the results of this method agree with the physical expectations, but more analysis is required in order to ensure that the method will always converge to the physical solution;
5. this method will be useful when using non-equilibrium Green's functions to model nanoelectronic devices that cannot have their Hamiltonians reduced to only the transport direction due to asymmetry in the device structure or the atomic positions, such as in the case of CNFETs without cylindrical gate electrodes.

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