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# Comparison of quantum mechanical methods for the simulation of electronic transport through carbon nanotubes

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ABSTRACT

In the present work we study the electronic transport properties of finite length single-wall carbon nanotubes (CNTs) by comparing three different theoretical frameworks. A simple model is used to describe the electrodes and the way they are attached to both ends of the CNT. Electron transport calculations are carried out on three different levels of sophistication. That are the Landauer transport formalism in combination with single-orbital tight-binding, extended Hückel theory or density functional theory. The quantum mechanical transmission which plays a central role in Landauer theory is calculated by means of equilibrium and non-equilibrium Green's function methods. Results of the three approaches are compared and discussed.



## 1. Introduction

During the last decades, semiconductor industry was driven by a continuous pressure in producing more powerful hardware. This was achieved by an exponential decrease of the minimum feature sizes within a microchip (Moore's law), now reaching dimensions where quantum effects play an important role. Special challenges arises from the down-scaling of conventional copper interconnects, as can be seen in the International Technology Roadmap for Semiconductors (ITRS) [1]. The resistivity is strongly increasing due to surface and grain boundary scattering and there are reliability issues due to electromigration when applying higher current densities [2].

Carbon nanotubes are thermally and mechanically stable while carrying high current densities [3], eliminating the electromigration problem that plagues copper. It is thus desirable to replace copper lines by CNTs (perhaps multi-walled or bundles) in future devices [4]. Besides other issues, like the reliable growth of highly aligned CNTs with a low defect density, the performance of such a device strongly depends on the quality of the contacts between CNTs and metal electrodes. Beside interconnect technology, CNT-based sensors are a growing field [5]. However, in both applications contacts between different CNTs or between CNTs and metal lines must be formed, having a strong influence on the performance of such devices.

Classical semiconductor device simulations are usually based on continuum models, neglecting the detailed atomic structure of matter and treating the current as a flow of charge carriers governed by Boltzmann's transport equation, for which various levels of approximations exits (like the drift–diffusion model, the hydrodynamic model, or the Monte Carlo method). When device dimensions are reduced towards the mean free path of the charge carriers, such descriptions break down and the quantum mechanics must be taken into account explicitly. This is can be achieved by a coupled solution of Schrödinger's and Poisson's equations (e.g. [6]) or by incorporating quantum corrections into classical approaches. However, if the detailed microscopic structure of a device shall be considered (like at the interface between a nanotube and some contacts), or for a true *ab initio* description of charge transport, atomistic methods are inevitable.

In the present paper we study electron transport in a finite-sized CNT attached to semi-infinite CNT-electrodes of the same geometry, applying and comparing three such methods. Despite its simplicity, this model has the main ingredients for a conceptual study on quantum transport through CNTs. The current through such device is calculated using the Landauer formula in combination with equilibrium and non-equilibrium Green's function methods for the quantum mechanical transmission. The goal is to compare different formalisms, namely single-orbital orthogonal tight-binding (OTB), extended Hückel theory (EHT) and density functional theory (DFT) for the description of the electronic structure of CNTs. The latter one, being an ab initio method, is highly predictable and transferable because, apart from the atomic arrangement, no further knowledge about the problem at hand is necessary. The drawback of DFT is its high computational cost. On the other hand, semiempirical methods like tight-binding (TB) and EHT are much less demanding, but results depend on

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external parameters that need to be fitted to reproduce properties known form experiments or other calculations. However, the accuracy can be comparable to first-principles calculations but transferability to different structures must be examined carefully. The present work can be seen as such an investigation.

Numerous studies about the electronic structure of CNTs and the junction to different electrodes have been made [7], applying empirical [8,9], semiempirical [10,11] and first-principle calculations [12–15]. Recently, we have reported OTB based transport calculations of metallic CNTs, comparing a contact model with structureless electrodes, as proposed by Nemec et al. [16,17], to the contact model used in the present work [18].

## 2. Model system

Quantum transport is a field of active research and computational approaches are quite demanding. With an application towards CNTs for interconnects in mind, it would be desirable to model a CNT in contact with metal electrodes (e.g. copper). However, this introduces complicated contact geometries and lifts the number of atoms within the whole calculation well above the number of CNT atoms. As the goal of the present work is a comparison of different computational approaches, we introduce simplified atomistic model as sketched in Fig. 1. A finite sized CNT (conductor) of length $L$ is in contact with two semi-infinite CNTs (electrodes) of same geometry. When a bias voltage is applied, current will flow from the left electrode through the conductor to the right electrode. The geometry of a CNT is defined by the binding length $d_{CC}$ of neighboring carbon atoms and the chiral vector $(M,N)$. We study the $(M,N) = (6,0)$ zigzag CNT with $d_{CC} = 1.42$ Å as in graphene. The length of the finite conductor is set to $N_{uc} = 5$ unit cells, which is equal to $L = 2.1$ nm. To investigate the influence of non-ideal contacts, the distance $d$ between conductor and electrodes is varied. It is important to note, that it is not possible to include the distance $d$ directly into the OTB framework, where a variation of the contact strength is achieved by changing the hopping parameter $\gamma_{cL/cR} \neq \gamma_0$ at the electrode–conductor interface.

Although being somehow artificial, this model captures essential transport properties of finite-sized CNTs. It is therefore a useful testbed for the applicability and performance of the three approaches in order to perform simulation on more realistic CNT devices.

## 3. Theory

In order to simulate a current flow through nanoscopic devices such as short CNTs, quantum mechanical methods have to be used. The task can be divided into electronic structure and transport calculation. Currently the "standard approach" is a self-consistent combination of density functional theory (DFT) and non-equilibrium Green's function methods (NEGF). Since this level of theory is relatively new in the field of microelectronics device modeling, we will explain the theoretical concepts in detail. The other two electronic structure methods, we use for comparison, are also briefly sketched.

### 3.1. Green's function methods for quantum mechanical transport calculations

A treatment of electronic transport on a molecular scale often starts with the Landauer formula $G = G_0 T(E = E_F)$ which links the conductance $G$ of a nanodevice at zero temperature and zero bias voltage to the quantum conductance $G_0 = \frac{2e^2}{h}$ and the total transmission probability $T(E = E_F)$ of electron waves at the Fermi energy [19]. The transmission function $T(E)$ and thus the value $T(E_F)$ depends on the geometry of the conductor and its coupling to the electrodes as discussed later.

The simple Landauer approach can be extended to both finite temperature and finite bias voltage. Assuming that the electrons within the left ($L$) and right ($R$) electrodes are in thermal equilibrium, their states are filled according to Fermi functions

$$f_{L/R}(E) = \{1 + \exp[(E - \mu_{L/R})/k_B T]\}^{-1}, \tag{1}$$

where $\mu_{L/R}$ are the chemical potentials of the left and right electrode. At zero bias the whole device is in equilibrium $\mu_L = \mu_R = E_F$. Applying a finite voltage $V_b > 0$ shifts the chemical potentials, which in case of a symmetric two terminal setup, as shown in Fig. 1, leads to

$$\mu_{L/R}(V_b) = E_F \pm \frac{eV_b}{2}. \tag{2}$$

Furthermore a finite bias induces an electric field that drives the system out of equilibrium, into a steady state, where electrons are constantly entering the conductor from left electrode and leaving to the right electrode. Net charge and electrostatic potential along the conductor will change and thus $T(E) = T(E,V_b)$ is a bias-dependent quantity. Finally, it has been shown that the current $I_{L\to R}$ is given by [20]

$$I_{L\to R}(V_b) = -\frac{2e}{h}\int (f_L(E,V_b) - f_R(E,V_b)) T_{L\to R}(E,V_b)\ \mathrm{d}E. \tag{3}$$

The remaining problem is how to calculate the transmission function.

In some localized non-orthogonal basis set, the Hamiltonian $H$ and overlap matrix $S$ for the whole system is made up of several blocks describing the subsystems (left electrode $L$, conductor $C$, right electrode $R$) and their coupling ($LC$, $RC$). We assume no direct coupling between the electrodes. This is strictly fulfilled within a localized basis, provided the conductor is large enough.

$$H = \begin{pmatrix} H_L & H_{LC} & 0 \\ H_{CL} & H_C & H_{CR} \\ 0 & H_{RC} & H_R \end{pmatrix} \tag{4}$$

The overlap matrix $S$ has exactly the same shape. It is important to note, that only the central part $H_C$ is finite while the semi-infinite electrodes are described be infinite sized matrices. We will now show, how the infinite problem can be reduced to a finite one by introducing the retarded Green's function $G^r$.

$$(\varepsilon^+ S - H) G^r = \mathbf{1} \tag{5}$$

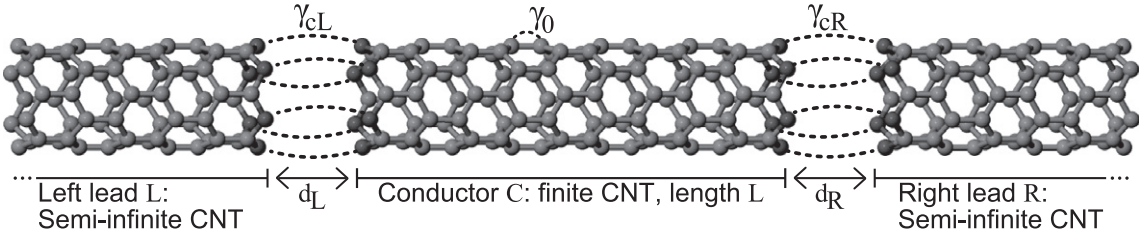


**Fig. 1.** Finite-sized central CNT of length $L$. The electrodes are modeled as semi-infinite CNTs having the same geometry as the center.