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Transport properties of a nanotube-based transistor

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Abstract. Transport properties of doped nanotube-based double junctions forming a nanotransistor are investigated within the tight binding formalism. The effects of doping, gate length and gate-source hopping have been considered. It is found that in addition to the importance of rotational symmetry in determining transport properties, large gains can be achieved for semiconducting doped tubes.

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1 Introduction

In this paper, we investigate the conduction properties of such tubes used as transistors in a setup where a bias is applied at the two ends playing the role of source and drain, and the central region submitted to a gate voltage by an STM tip for instance. The effect of such a tip would be to raise or lower the electrostatic potential of the gate region, thus forming two junctions. The effect of doping is also investigated as in usual transport measurements, where the tube is deposited on a substrate, and there can be some charge transfer from substrate to the tube. In our previous work, we have studied the electronic and transport properties [1,2] of a single junction within the self-consistent tight binding formalism. Our purpose here is to study qualitatively the effects of the gate length and doping on the conductance as a function of the gate voltage and show that by tuning the latter, the device can function as a transistor.

Let us consider an infinitely long nanotube formed of 3 parts: the left semi-infinite part attached to a reservoir of chemical potential μ_L, the right semi-infinite part attached to a reservoir of chemical potential μ_R, and the central part attached to a gate of potential V_G. The thickness of the gate region is variable. For simplicity, we will assume the left and right parts to be identical, and having the same chemical potentials. We will be at first interested in the conductance of this device as a function of the gate voltage. In a second part, we will consider the left and right parts as doped. This in effect will shift the chemical potential, and thus the occupations of the sites. This shift is due to charge transfer coming from doping which could either be dopant atoms inside or outside the nanotube, or just a contact with a substrate of different work function.

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2 Method

The system is described with a tight-binding Hamiltonian with only one π orbital per atom. This Hamiltonian can describe reasonably well the band structure of a nanotube especially near the Fermi level which is zero in this case since the onsite energy is assumed to be zero, and each orbital is half-filled;

$$\mathcal{H} = \sum_i \epsilon_i c_{i\sigma}^\dagger c_{i\sigma} + t \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma}. \quad (1)$$

The on-site energy ϵ_i will be set to zero in a first place, except in the gated region where it is equal to V_G. In this case, the Fermi level of the two leads is also equal to zero. In this work, the effect of self consistency has been dropped for simplicity as it does not affect qualitatively the transport phenomena in nanotubes. Our calculations have shown that the screening is short-ranged with small oscillations for large steps in the junction potential.

The retarded and advanced Green's functions (GF) are defined as:

$$G^{r/a}(E) = [E - \mathcal{H} \pm i\eta]^{-1}, \quad (2)$$

where η is a small positive number, and + (resp. −) corresponds to the retarded (resp. advanced) GF. This operator is defined in the space spanned by all the orbitals of the nanotube. We need, however, its projection in the gated region. This is defined by a matrix:

$$G_{ij}(E) = \langle i|G(E)|j\rangle,$$

where i and j are two orbitals belonging to the gated region. One can show that these matrix elements, can be obtained from the following relations [3] which can be derived using the partitioning technique:

$$G^{r/a}(E) = [E - \mathcal{H}_{gate} - \sum_{\alpha} \Sigma_{\alpha}^{r/a}(E) \pm i\eta]^{-1}, \qquad (3)$$

where the self energy matrix Σ_{α}, representing the effect of the lead α on the gate, is defined by:

$$[\Sigma_{\alpha}^{r/a}(E)]_{ij} = \sum_{kl} H_{ik}\, [g_{\alpha}^{r/a}(E)]_{kl}\, H_{lj}, \qquad (4)$$

the index α being any of the contacts to the gate (Left or Right), i and j label two sites of the gate, and k and l belong to the lead α. g is the GF of the isolated semi-infinite left or right lead. In practice, it is projected on the last layer of the lead, and hence it is really a surface GF. It can be computed separately by iterative methods [4]. The conductance of the whole system can then be computed from the Landauer formula derived first for interacting systems by Meir and Wingreen [5]:

$$\mathcal{G}(E) = \frac{2e^2}{h} \mathrm{Tr}\left(G^r(E)\Gamma_L(E)G^a(E)\Gamma_R(E)\right), \qquad (5)$$

where the transition rate matrix Γ is $-2\mathrm{Im}\Sigma$. For a large gate region, the most time consuming part of the program is the matrix inversion in Eq. (3), which can be made more efficient (proportional to the length of the gate) for one-dimensional systems.

3 Results and discussions

We first studied the effect of lead to gate hopping. In the case of a nanotube gated by an STM, the hopping stays uniform all along the tube, and therefore this effect does not occur. In general, however, if one is dealing with a "quantum dot", the strength of hopping will affect the conductance since the latter is proportional to the fourth power of lead-dot hoppings (see Eq. (5)). It was observed that a smaller hopping would reduce the conductance to very small values except for energies exactly equal to the dot's eigenvalues where there would be resonant transmission. With weak couplings to the leads, one could thus perform spectroscopy of the energy levels of the dot.

We next set $\epsilon = 0$ for the left and right leads, and $\epsilon = V_G$ in the gated region, and compute the conductance as a function of the gate voltage for gates of various lengths in a $(4,4)$ armchair nanotube. For a semiconducting zigzag nanotube, the density of states (DOS), and therefore the conductance at the Fermi energy $E_F = 0$ is always zero. The results for gates formed of 2, 4 and 8 layers of carbon rings in a $(4,4)$ armchair tube are displayed in Fig. 1.

One notices that the number of oscillations increases with the length of the gated region. The peaks can be understood in terms of resonant transmission through the gated region. Every time the Fermi energy is such that the width of the gate is a multiple of the incoming electron wavelength, there is resonant transmission (transmission probability = 1) and the conductance peaks at that energy. The number of peaks naturally increases as a function of the length of the gate.

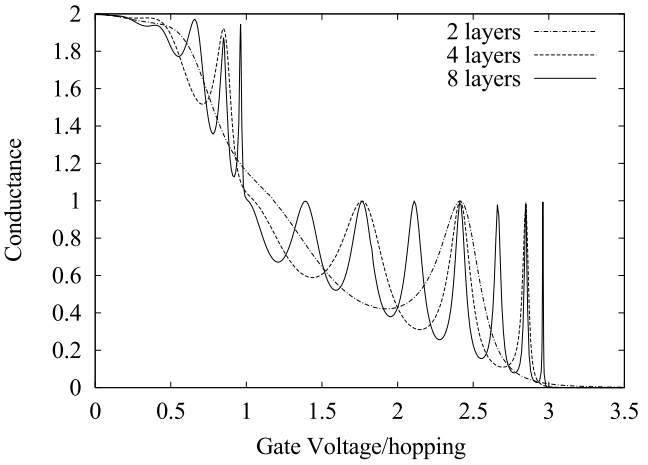

Fig. 1. Conductance of a 2 layer, a 4 layer and a 8 layer gated region *versus* the applied gate voltage in a $(4,4)$ armchair nanotube. The curve is even in V_G since the DOS of the nanotube is even in energy.

The other important feature noticeable in this curve is the reduction of the conductance envelope from 2 to 1 as the gate voltage becomes larger than the hopping integral t. This phenomenon is due to the rotational symmetry of the tube. In the gated region, one can assume that the local DOS is shifted with respect to the leads by V_G. In this case, for $V_G > t$ the number of "s" channels at energy 0 is decreased from 2 to 1, as the number of right moving s channels of energy 0 in the leads is equal to 2. Therefore, the conductance is reduced by one (in units of $2e^2/h$) as V_G becomes larger than t. This phenomenon was also observed in the study of nonlinear transport in single n-p junctions [2], and is solely due to the rotational symmetry selection rule. It is anticipated that a small asymmetry in the onsite energies due to a contact with a substrate for example will not affect this change in the conductance much, since that would only slightly change the shape of the "s" states and not their phase.

We then focus our attention on the doped case, *i.e.* consider a non-zero chemical potential, and perform the same calculation of the conductance. This study can also be performed for zigzag nanotubes since there would be a non-zero DOS at the Fermi level in the two leads. The results are summarized in Fig. 2 for the $(4,4)$ armchair, and Fig. 3 for the $(7,0)$ zigzag tube.

One can notice a large change in the conductance of both devices for some values of the gate voltage. This effect is more pronounced in semiconducting tubes as their DOS is zero in some energy range. The conductance changes by a factor of 30 as V_G goes from 0 to 0.95 hopping in the high doping limit ($E_{\mathrm{F}} = 0.99$) and even by a much larger factor of 440 for $E_{\mathrm{F}} = 0.25$!

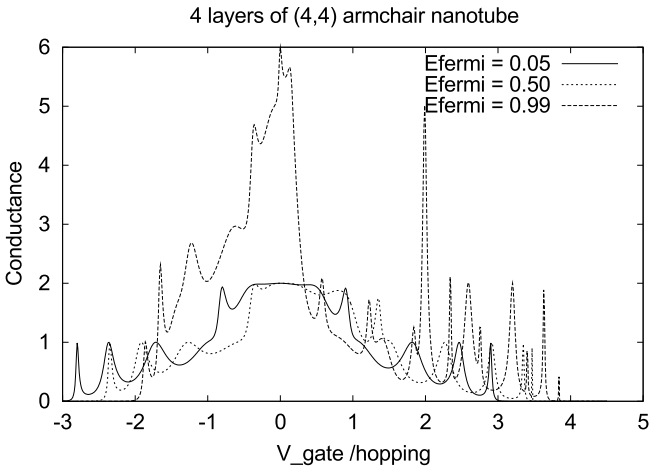

Fig. 2. Conductance of a 4 layer gated region *versus* the applied gate voltage in a $(4,4)$ armchair nanotube for several Fermi energies.

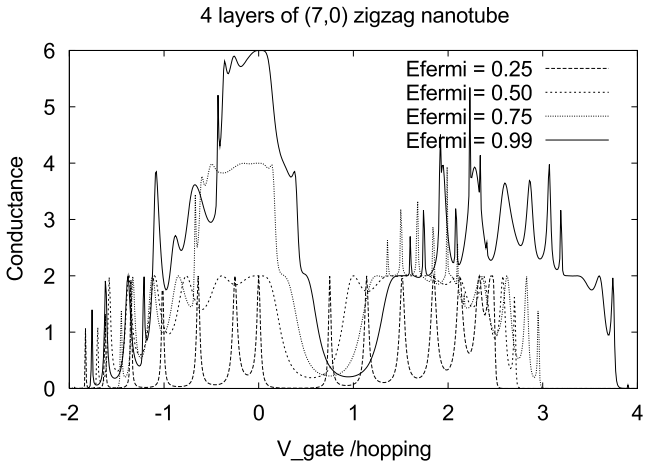

Fig. 3. Conductance of a 4 layer gated region *versus* the applied gate voltage in a $(7,0)$ zigzag nanotube for several Fermi energies.

4 Conclusions

In conclusion, the rotational symmetry of the tube is an important factor in determining its transport properties. Semiconducting tubes are good candidates for making nanotransistors out of doped nanotubes where we have observed that gains of about 400 or more can be achieved.

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