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Rotational Symmetry Selection Rule and Doping in Nanotube Transistors

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We consider a nanotube with its central part attached to a gate region of variable potential and variable length. This device can work as a nanotransistor in the sense that the gate voltage controls the current across the tube. Using Landauer formalism, the conductance of this device is calculated as a function of the gate voltage. For wider gate regions, the conductance shows an oscillatory behavior reminiscent of resonant transmission. A half reduction in the conductance can be noticed if the gate voltage differs with the Fermi energy of the leads by more than a hopping integral. This effect is associated with the rotational selection rule allowing only transmission to channels with the same angular momentum. From these calculations, one can also deduce the conductance of a magnetically doped tube or one connected to ferromagnetic leads.
Key words : nanotube, transport, transistor, doping

1.INTRODUCTION

In this paper, we study the conduction properties of carbon nanotubes used as transistors in a setup where a bias is applied at the two ends playing the role of source and drain. The central region is weakly coupled to a gate. The gate could be 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 properly tuning the latter, the device can function as a transistor.

We 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.

2.MODEL AND CALCULATION 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;

$$H = \sum_i \varepsilon_i c_i^+ c_i + t \sum_{<ij>} c_i^+ c_j$$

In what follows, all energies will be in units of t=2.7 eV. 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. A weak coupling to the gate is assumed so that leak currents to the gate are neglected. Furthermore, we assume strong coupling of the gated region to the rest of the system considered as leads.

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

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

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:

$$G_{ij}(E)=<i|G(E)|j>$$

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:

$$G^{r/a}(E)=[E-H_{gate}-\sum_{\alpha}\Sigma_{\alpha}^{r/a}(E)\pm i\eta]^{-1} \quad (1)$$

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

$$[\Sigma_{\alpha}^{r/a}(E)]_{ij}=\sum_{kl}H_{ik}[g_{\alpha}^{r/a}(E)]_{kl}H_{lj} \quad (2)$$

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]:

$$G(E)=\frac{2e^2}{h}Tr[G^r(E)\Gamma_L(E)G^a(E)\Gamma_R(E)]$$

where the transition rate matrix Γ is -2 Im Σ. For a large gate region, the most time consuming part of the program is the matrix inversion in Eq. 1, which can be made more efficient (proportional to the length of the gate) for one-dimensional systems.

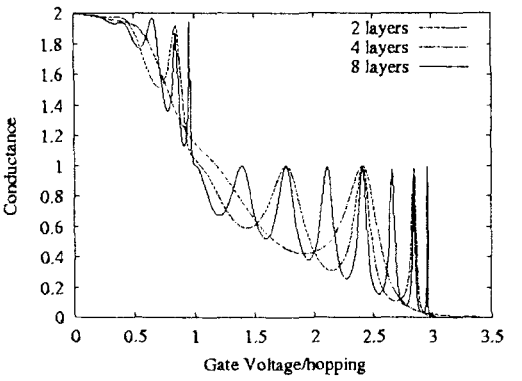

Figure 1: Conductance of a 2 layer, a 4 layer and a 8 layer gated region versus the applied gate voltage in a (4,4) armchair nanotube. The curve is even in V_G since the DOS of the nanotube is even in energy.

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 hopping (see Eq. 2). 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. In this case, the calculations need to be self-consistent in order to properly take into account of dot charging and thus Coulomb Blockade effects.

We next set $\varepsilon=0$ for the left and right leads, and $\varepsilon=V_G$ 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.

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 channels of "s" symmetry, i.e. with angular momentum L_z=0, at energy 0 is decreased from 2 in the leads to 1 in the gate, 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 2 e^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. Indeed that would only slightly change the shape of the "s" states and not their phase, and therefore the scattering from an "s" channel to a "p" channel would be come very small under the asymmetry.

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 Figs. 2 for the (4,4) armchair, and 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 the LDOS in the gate could be zero for appropriately chosen gate voltages. In the (4,4) armchair tube, the conductance can change from 6 to 0.2, i.e. by a factor of 30 as V_G

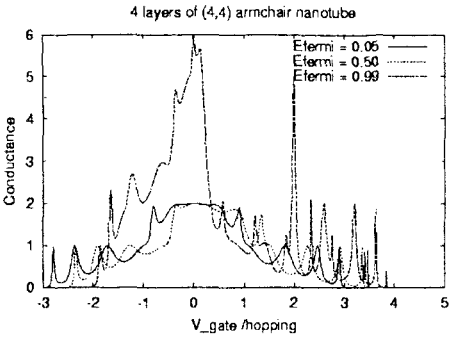

Figure 2: Conductance of a 4 layer gated region versus the applied gate voltage in a (4,4) armchair nanotube for several Fermi energies.

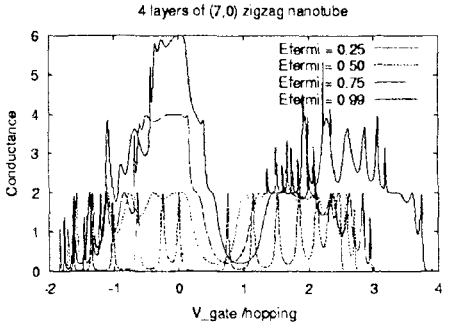

Figure 3: Conductance of a 4 layer gated region versus the applied gate voltage in a (7,0) zigzag nanotube for several Fermi energies.

goes from 0 to 0.95 hopping in the high doping limit E_F=0.99. Interestingly, for the semiconducting (7,0) tube, and at E_F=0.25, the conductance can vary from 1 to almost 0. The actual gain is a factor of 440, as the LDOS in the gate is not exactly equal to zero.

For tubes doped with magnetic elements, or deposited on a magnetic substrate, the situation becomes interesting. Indeed we discover a spin valve effect. When the magnetization of the two leads is parallel the conductance as a function of the gate voltage is similar to the above curves, though not exactly the same. The magnetic dopants cause the up-spin band and the down-spin bands to split, so that due to the different DOS for the two spin values, one obtains a magnetic current. If the magnetization of the two leads have opposite directions, the splittings have also different directions in the two leads. This usually leads to a decrease in the conductance compared to the parallel case. The ratio of

the two conductances is, however, usually a fraction of 1, but not very small. In the case of the nanotransistor, the freedom in playing with the gate voltage allows the LDOS of this region to have values raging from 0 to very large numbers, thereby allowing one to control the conductance of the device. It was found that if the lead regions are undoped, the conductance ratio does not change drastically with the gate voltage. But when the leads are doped, and the Fermi energy moves in the VanHove singularity region for instance, where the DOS is largest, this ratio can become very small.

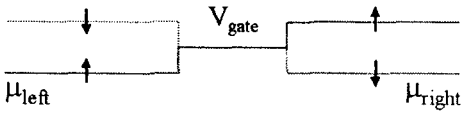

Figure 4: Schematic representation of the conduction channels in the antiferromagnetic configuration.

We compare in Fig. 5 the conductance of parallel and antiparallel configurations as a function of the gate voltage. The strong spin valve effect can be observed in this case for gate voltages of 2t or larger where the conductance of the antiferromagnetic configuration is almost 0. In this calculation a up-down splitting of

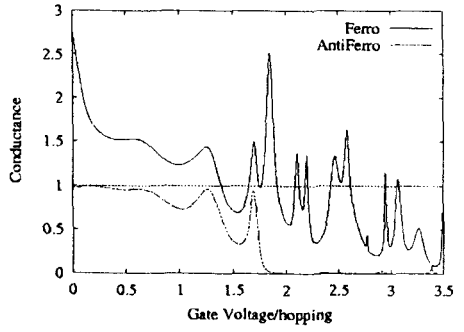

Figure 5: Effect of magnetic dopants on the conductance of a (4,4) armchair tube. E_F=0.85

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. A strong spin valve effect can be achieved for appropriately magnetically doped leads.

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