Nonlinear effect in conductance of a finite-length armchair single-wall carbon nanotube due to presence of a single impurity

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Abstract. We have theoretically investigated the first correction to quantum conductance of finite Single-Wall Carbon Nanotubes (SWCNT) due to presence of a single impurity. We have tried to analytically obtain the change in the conductance of a SWCNT, by means of a perturbative scheme along with finite-length real space nearest neighbors tight binding method for carbon $\pi$-orbitals. Dependence of the differential conductance on source-drain voltage as well as its sensitive dependence on the position of the possible impurity/defect on the tube is studied. Results suggest a promising method for spectroscopy of electronic energy levels and imaging accurate position of carbon atoms in a SWCNT.

Recent developments in carbon naotubes fabrication techniques open a new horizon in technology of electrical devices [1]. A SWCNT can be considered as a graphene sheet folded around a specific axis. Almost one third of these structures are conductors [2]. Conductance of an ideal SWCNT is $G_0 = 4e^2/h$ [3] (and references therein). Meanwhile, presence of any kind of disorder or imperfection in these structures will affect the conductance [4]. These disorders are always present. As an special case some desirable or undesirable non-carbon atoms on the surface of the tube are present [5]. In this case, unlike the bulk conductors, presence of a single impurity will dramatically change the conductance. The more interesting point is that the conductance is not only dependent on the number of such single defects, but also on the position of them. Using well-known techniques [6] now researchers are able to cut nanotubes into segments in length of a few tens of nanometers. This produces new electronic properties for finite-length carbon nanotubes: Confinement of the length results in completely quantized energies for conduction electrons - confirmed by experiment [7] - and makes the probability of finding electrons be different from one point to another along the nanotube, which is essential in understanding the size effects. Obviously, it is important to study such quantum size effects in view of the device application of nanotubes. By now, different studies have focused on electronic properties of finite-length carbon nanotubes [8].

In this research we considered only one single impurity (or defect) on the surface of a finite metallic SWCNT. We tried to analytically obtain the change in the conductance of a SWCNT, due to the presence of a single impurity/defect, by means of finite-length $\pi$-orbital tight binding method in real space for including tube length. As it will be expressed, for a limited length
carbon nanotube, amount of scattering of the conduction electrons’ wave functions from a defect (and as a result a change in the conductance of the nanotube) depends on the position of the possible defect. We have tried to investigate this dependence as well as nonlinear part of conductance. We see that our results introduce a quantitative method for spectroscopy of the energy levels as well as imaging the relatively accurate position of carbon atoms on surface of the tube by analyzing the superposition of electronic intensities corresponding to states near the Fermi level. This is what can be investigated by Nano-probes as a causer of such point-like defects.

Let us consider a metallic SWCNT as a long but finite cylinder, which connects two bulk metallic electrodes. Assuming the nanotube to be long assures us that electric field inside the tube and far from its two ends is negligible and energy of ballistic electrons depend only on the sign of their velocity. The electrodes lie in different voltages $V_i$, assuming $eV \ll E_F$. We also assume that a single impurity/defect is located on the surface (or is slightly displaced from the surface) of the cylinder. We will completely neglect possible backscattering of electrons on metal contacts. The Hamiltonian of the electrons, $H$, contains following terms:

$$H = H_0 + H_1 + H_{int}$$

where

$$H_0 = \sum_k \varepsilon_k c_k^\dagger c_k$$

is Hamiltonian of Bloch electrons feeling only perfect lattice of SWCNT,

$$H_1 = \frac{eV}{2} \sum_k \text{sgn}(v_z) c_k^\dagger c_k$$

describes the interaction of the electrons with the electric field. Here operator $c_k^\dagger(c_k)$ creates (annihilates) a conduction electron with wave function $\Psi_k$ and energy $\varepsilon_k$. As will be seen later, $k$ is the full set of electron’s quantum numbers for translational and rotational degrees of freedom (ignoring spin). $v_z$ is the electron velocity along the tube axis. Finally $H_{int}$ is the Hamiltonian of interaction between electrons and single point-like impurity located at $r$:

$$H_{int} = g \sum_{k,k'} \Psi_k(r) \Psi_{k'}^*(r) c_k^\dagger c_k$$

The strength of this interaction, $g$, is assumed to be small. The conductance of the system is described by the Landauer formula [9], which is applicable if the wave function can spread over the whole sample. Using second quantized representation for Hamiltonian and a perturbative scheme, we can investigate the influence of aforementioned single impurity/defect to the first order. The rate of energy dissipation due to presence of the impurity/defect can result in a change in the electric current [10, 11]. Here we assume that we are working in zero temperature, so Fermi distribution function which controls the accessibility of injected electrons by reservoirs turn out to be Heaviside step function. By some tedious algebra we can get an analytic form for first correction to quantum conductance due to presence of a single impurity/defect [12, 13]

$$G_1 = G_0 \left( \frac{g \pi}{2} \right)^2 \sum_{i,j} (\text{sgn } v_{z_i} \text{sgn } v_{z_j} - 1) \delta(E_F - \varepsilon_j - \frac{eV}{2} \text{sgn } v_{z_j})$$

$$\times \delta(\varepsilon_j - \varepsilon_i) [\Psi_i^2(r) \Psi_j^2(r)]$$

We refer to $E_F$ as the common chemical potential of the whole system including both nanotubes and reservoirs. For a typical nanotube summation over $i$ (or $j$) stands for all quantum numbers.
There are three factors in equation (5): I. the velocity of carriers within the bands; II. the strength of interaction or which determines the quantum interaction effects; and III. the type of band structure.

Here for calculating the wave functions and energies for infinitely long SWCNTs finite-length real space π-orbital Tight-Binding (TB) method for graphene sheet along with zone-folding approximation has been used. In the case of finite-length tubes, electronic wave vectors corresponding to electrons’ translational degree of freedom along the tube axis are also discrete and along with already quantized wave vectors along the circumference of the tube build up a completely quantized electronic states. Tube axis is assumed to be along z-axis. We have also used a SIESTA code [14] to obtain the radial part of carbon 2p_z orbitals. Our formalism introduced in this section is applicable to metallic structures.

Figure 1 shows first correction to the conductance, G_1, versus source-drain voltage for (5,5) armchair tube of length 88T where T is the translational period along tube axis. The vertical axes in figures 1 and 2 are scaled in such a way that we have \((g_m/e\bar{h}) \times 10^{-4} = 1\). In (b) the length of the tubes is altered to show the length dependence. Lower panel in both (a) and (b) is the finite-length band structure of corresponding tubes in energy range of applied voltage: 0 to 1eV. In this energy range only one band contributes to the conductance. Two graphs are plotted for three different impurity/defect positions on surface of the tube and source-drain voltage runs from zero to 1eV. As the length of tube increases number of allowed states and number of peaks in G_1 graph also increase. G_1 is sensitively dependent on the position of the impurity/defect on the tube along its axis. As voltage is raised from 0 to 1eV, graph shows pair of peaks in G_1 in figure 1. Sensitive dependence of G_1 on impurity position is clear in the upper panels. A peak occurs just when an electronic state contributes to the conductance as the voltage rises. In fact, this graph is qualitatively similar to local density of states (LDOS) of the tube in hand. Thus, calculating the first correction to the conductance provides a promising method for spectroscopy of energy levels in the nanotube [15]. Heights of the peaks sensitively depend on the position of the impurity/defect. For the second lower panel in figure 1(a) and (b), in which the impurity/defect is assumed to be placed on the middle of the tube, all peak heights are almost equal since the middle point is a point where a carbon atom dwells and has maximum intensity. Also, height of the peaks are decreased in figure 1(b) in comparison with (a) since on the overall value of TB wave functions is also decreased by normalization factor. However, the number of allowed states are increased but, as is clear from figure 1(b), the dominant factor is...
normalization factor and \( G_1 \) decreases as the tube length is increased.

Figure 2 shows \( G_1 \) as a function of impurity/defect position along tube axis for a (10,10) tube of length 28\( T \). \( G_1 \) graph has oscillatory behavior just as was expected [15]. The line scan along the tube axis is picked in such a way that the environment is almost the same for tubes with either even or odd indices and is identical to line scan indicated in the inset. Maxima occur just when the impurity/defect is situated above a carbon atom. The pattern here is a measure for sum of electronic wave function intensities near the Fermi level along a specific line scan. By smoothly moving the line scan along the circumference we can get points where the peaks occur throughout the tube and then we can obtain the exact position of carbon atoms on the surface of the tube. The procedure can be used as an imaging method for electronic intensities as well as determining almost exact position of carbon atoms. Dotted line in figure 2 shows \( G_1 \) versus impurity/defect position for a (5,5) tube of length 28\( T \). Magnitude of \( G_1 \) is notably larger in (5,5) tube case. As the index of the tube increases, normalization factor lowers the overall value of each electronic wave functions all over the tube and \( G_1 \) increases as the diameter is decreased. Moreover, figure 2 also shows edge effects.

To summarize, the effect of a single defect on the differential conductance of a finite-length armchair SWCNTs within the context of perturbation scheme, is studied. Our results show that there is an interplay between position of the defect, the length and the diameter of the tube which affect the value of differential conductance. Moreover, results show a potential application of a new spectroscopy method for electronic energy levels in metallic SWCNTs and imaging the almost exact positions of carbon atoms on tube surface.

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