Differential conductance of armchair single-wall carbon nanotubes due to presence of electron–phonon interaction

Fatemeh Tajik [a,*], Afshin Namiranian [b,c]

[a] Department of Physics, Alzahra University, Vanak, 1993891167 Tehran, Iran
[b] Department of physics, Iran University of Science and Technology, Narmak, 16345 Tehran, Iran
[c] Computational Physical Science Laboratory, Department of Nano Science, Institute for Research in Fundamental Sciences(IPM), P.O. Box19395–5531, Tehran, Iran

HIGHLIGHTS

- It is theoretically presents the effect of electron-phonon interaction on the conductance of armchair single-wall carbon nanotubes by using a perturbative method.
- The influence of radial breathing mode and tangential optical mode are investigated on the conductance pattern of armchair single-wall carbon nanotubes.
- The dependence of differential conductance on tube length and diameter is studied.

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ABSTRACT

We have theoretically investigated the first correction to conductance of armchair single wall carbon nanotubes (SWCNTs) with finite length, embedded between two electrodes, due to the presence of electron–transversal phonon interaction. The perturbative scheme has been used with finite length real space nearest neighbors tight binding method. Both radial breathing and tangential modes are investigated separately. It is found that not only the conductance correction crucially depends on source-drain voltage but also it strongly depends on the length and diameter of SWCNT. So, this work opens up opportunities to control the electrical conductance of SWCNT and increases yield of micro or nanodevices based on carbon nanotube.

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1. Introduction

During the last few decades, there has been much interested in carbon nanostructures. These structures have been able to make a big evolution in technology of electrical devices [1]. A single-wall carbon nanotubes (SWCNT) is a sheet of honey-comb lattice of carbon atoms rolled up to be a cylinder [2]. One third of these structure are conductors [3]. The conductance of an ideal SWCNT is, $G_0 = \frac{(4e^2)}{h}$ [2,4]. Meanwhile electron–phonon interaction is one of the main sources of electrical resistance in a conductor [5]. This fact is observed experimentally and already has been verified that scattering of electrons from phonons may remarkably change electrical conductance inside a not so long SWCNT [6,7]. Several theoretical investigations have been devoted to explain different aspects of the electron–optical phonon interaction in SWCNTs, mostly focusing on electron–longitudinal phonon interaction which has the dominant effect [8,9]. On the other hand, studies over behaviors of transversal phonons on a SWCNT are interesting, because they are important on characterizing a SWCNT for example on the Raman spectroscopy [8–12]. In Ref. [13], it is shown that the differential conductance of carbon nanotube depends on length and diameter of nanotube. In this research the change in conductance of a SWCNT due to the presence of electron–phonon interaction is obtained by using a perturbative method. It is demonstrated how strong dependence of electron–phonon interaction in carbon nanotube on characteristic quantities of nanotube (length and diameter) can cause intensive dependence of conductance pattern of SWCNT, which is due to electron–phonon interaction, on tube length and diameter. This dependency is investigated on radial breathing mode (RBM) and tangential optical mode (TO) in SWCNT.

The more interesting point is that the conductance not only dependent on electron–phonon interaction, but also is shown with

* Corresponding author.
  E-mail address: f.tajik@student.alzahra.ac.ir (F. Tajik).

a proper choice of SWCNT in nanodevices, it is possible to change the conductance pattern of nanodevices and increase its yield. This work opens up opportunities with available data of conductance pattern of multi SWCNT to recognize characteristic quantities of these nanotubes (length and diameter) in comparison with each other. The text is organized as follows: in Section 2, we briefly describe the model and method. We discuss our results in Section 3. Finally our conclusion is presented in Section 4.

2. The model

In our model we assume an armchair SWCNT, lying between two metallic electrodes (Fig. 1).

Voltage, V, is applied between the electrodes where $eV \ll \epsilon_f$, where ϵ_f is the Fermi energy of electrons in carbon nanotubes. In order to neglect the effect of the open ends of the nanotubes on the electrical resistance, we assume that the nanotube length is much longer than its diameter. Under this approximation, the electrical field inside the tube and far from its two ends is negligible and the energy of passing electron depends only on the sign of the electron velocity along the contact axis [13,14]. In this work, using second quantized representation for Hamiltonian, the total Hamiltonian of the entire system can be described in a general form, as follows:

$$H = H_0 + H_1 + H_{int} \tag{1}$$

The first term describes the energy of electron and phonon for a perfect SWCNT as follows:

$$H_0 = H_e + H_{ph} \tag{2}$$

$$H_e = \sum_k \epsilon_k a_k^\dagger a_k \tag{3}$$

$$H_{ph} = \sum_q \hbar\omega_q b_q^\dagger b_q \tag{4}$$

Second term, H_1, is considered for the interaction of electrons with the electric field and it represented by:

$$H_1 = \frac{eV}{2} \sum_k sign(v_{kz}) a_k^\dagger a_k \tag{5}$$

The last term is Hamiltonian of interaction of electrons with phonons. It can be written as follows:

$$H_{int} = \sum_{k,k'} M_{k,k'}(b_{k'-k}^\dagger + b_{k-k'}) a_k^\dagger a_{k'} \tag{6}$$

ϵ_k is the energy of Bloch electron. We have used the tight-binding method for graphene sheet, up to nearest neighbors interaction with zone folding approximation along the tube axis [15]. The operator $a_k^\dagger(a_k)$ creates (annihilates) a conduction electron with energy ϵ_k (k is quantum number of electron along the tube axis). The operator $b_q^\dagger(b_q)$ creates (annihilates) a phonon with energy $\hbar\omega_q$ (q is the quantum number of phonon). v_{kz} is the electron velocity along the length of CNT. $M_{k,k'}$ is the electron–phonon interaction matrix element. Here, we only focus on the electron–optical phonon interaction effects in optical tangential (TO) and radial breathing mode (RBM). The matrix elements of electron–phonon interaction are represented for an armchair SWCNT (m, m) by [16–18]:

$$M_{\vec{k},\vec{k'}}^{RBM} = |D| \sum_{k,n,k',n'} \sqrt{\frac{\hbar}{\omega_q M_u N_z}} \left(\cos\left(\frac{n\pi}{\sqrt{3}\,m}\right) + \cos\left(\frac{n'\pi}{\sqrt{3}\,m}\right) \right) \sin\left(\frac{\pi}{2\sqrt{3}\,m}\right)$$
$$+ \left(\cos\left(\frac{\sqrt{3}\,ka}{2}\right)\cos\left(\frac{n\pi}{2\sqrt{3}\,m}\right) + \cos\left(\frac{\sqrt{3}\,k'a}{2}\right)\cos\left(\frac{n'\pi}{2\sqrt{3}\,m}\right) \right)\sin\left(\frac{-\pi}{4\sqrt{3}\,m}\right) \tag{7}$$
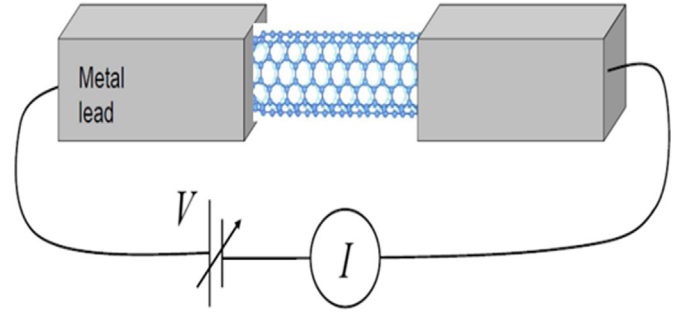
$$M_{\vec{k},\vec{k'}}^{TO} = |D| \sum_{k,n,k',n'} \sqrt{\frac{\hbar}{\omega_q M_u N_z}}\ times$$
$$- \left(\cos\left(\frac{n\pi}{\sqrt{3}\,m}\right) + \cos\left(\frac{n'\pi}{\sqrt{3}\,m}\right) \right)\cos\left(\frac{\pi}{2\sqrt{3}\,m}\right)$$
$$+ \left(\cos\left(\frac{\sqrt{3}\,ka}{2}\right)\cos\left(\frac{n\pi}{2\sqrt{3}\,m}\right) \right.$$
$$\left. + \cos\left(\frac{\sqrt{3}\,k'a}{2}\right)\cos\left(\frac{n'\pi}{2\sqrt{3}\,m}\right) \right)\cos\left(\frac{-\pi}{4\sqrt{3}\,m}\right) \tag{8}$$

M_u is mass of unit cell of CNT. N_z is the number of atomic layers along the nanotube axis. a is the nearest neighbors distance between two carbon atoms. D is the deformation potential. In our calculations, D is taken to be 6 eVÅ^{-1} [16]. ω_q ($q = k - k'$) represents phonon frequency. $n(n')$ is the quantum number of electron along the circumference of tube before (after) scattering. In order to keep our perturbation scheme of calculation valid, we assume that only conduction and valance bands contribute in conductance. In this study, we have used the result of Mahan and Jeon work [16–18]. They utilized the force constant method to obtain phonon dispersion of armchair SWCNT. In order to investigate the influence of electron–phonon interaction on conductance of CNT, we have used a method based on the perturbation theory which was developed by Kulik et al. [19]. In this method, change of electrical current, I, due to the electron–phonon interaction is connected with the rate of dissipation of the energy, E, as

$$V\Delta I = \frac{dE}{dt} = \frac{d\langle H_1 \rangle}{dt} \tag{9}$$

By differentiating $\langle H_1 \rangle$ with respect to time, which is obtained from the Heisenberg equation, one can obtain ΔI as a result of the interaction of electrons with phonons:

$$V\Delta I = \frac{1}{i\hbar}\langle [H_1(t), H_{int}(t)] \rangle \tag{10}$$

where

$$\langle O \rangle = \mathrm{Tr}(\rho(t)O) \tag{11}$$

The statistical operator $\rho(t)$ (the density matrix) satisfies the equation:

$$i\hbar\frac{\partial\rho(t)}{\partial t} = [H_{int}(t), \rho(t)] \tag{12}$$

which can be solved by using an iterative scheme for $\rho(t)$:

$$\rho(t) = \rho_0(t_0) + \frac{1}{i\hbar}\int_{-\infty}^t dt'[H_{int}(t), \rho_0(t)] \tag{13}$$

Thus, the change in the electric current due to the presence of electron–phonon interaction can be determined as [14,20]:

Fig. 1. The model of an armchair SWCNT lying between two metallic leads.