Effect of Electron-RBM Phonon Interaction on Conductance of Metallic Zigzag Carbon Nanotubes

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We use the energy analysis as a perturbative method to study the effect of electron-radial breathing mode (RBM) phonon interaction on the electrical conductance of long metallic zigzag carbon nanotubes (CNTs). The band structure of zigzag CNTs is calculated by exerting zone-folding method on relations derived by using the nearest neighbor approximation of tight-binding expression for the π bands of graphene. The small hollow cylinder model, with two different approximations, is used to obtain the RBM frequency in our calculation. As the result, we have calculated the effects of electron–RBM phonon interaction on the conductance of zigzag CNTs. It has been observed that current is a step–like function of bias voltage due to the absorption or emission by electron injection in the system. Moreover, the dependence of the conductance to the temperature in low bias and high bias voltages has been studied. In this paper, we propose a simple and useful method for phonon spectroscopy. Also, since RBM mode determines the geometry and structure of CNT, this approach can be used for characterization of CNTs.

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I. INTRODUCTION

The appearance of carbon nanotubes\textsuperscript{1,2} (CNTs) as promising building blocks for electron flow have established a novel revolution in science and technology of nano–scaled devices. Since in comparison with other systems, scattering factors have less effect on CNT’s conductance, it becomes essential to perceive the electron transport properties of these quasi–one–dimensional systems\textsuperscript{3}. CNTs can be considered as a rolled graphene sheet which can be in the form of single–wall or multi–wall. Moreover, single–wall CNTs (SWCNTs) can be categorized into two forms of chiral and achiral tubes that the achiral ones are divided into zigzag and armchair. While armchair CNTs are metals, zigzag CNTs can be metal or semiconductor based on their geometry. In practice, in the production of CNTs, they would be produced with several diameter sizes together, so it would be important to propose a method to detect the CNT’s diameter size in the system.

CNTs demonstrate diverse significant properties\textsuperscript{4–8}, importantly, one of these remarkable properties is elevated conductance in the ballistic regime\textsuperscript{1}, as it has been shown that the current density of CNTs can reach near $10^9\, \text{cm}^2\, \text{s}^{-1}$. This, together with being quasi-one-dimensional system make CNTs a novel candidate to be used as metallic interconnecting systems (quantum wires)\textsuperscript{10–13}.

Beside their application as conducting wires\textsuperscript{14}, CNTs can be used as field–effect transistors\textsuperscript{15}, or single–electron–tunnelling transistors.\textsuperscript{16} Although, CNTs are good ballistic transport one can still consider several proposals for scattering in these materials. One of the main mechanisms is the electron–phonon (e–ph) interaction which is an important scattering mechanism in the CNTs for a wide range of temperatures.

Novel properties and one–dimensional structure of CNTs yield to emerge unique modes and properties in their phonon spectrum\textsuperscript{17}. Characterisation of CNTs has been done extensively by Raman spectroscopy\textsuperscript{18–22}, and Dependant on the type of vibrations of carbon atoms in a long CNT, three types of phonon modes exist: 1) RBM phonon mode that comes from coherent radial vibrations of carbon atoms; 2) Longitudinal phonon modes that are due to vibrations of carbon atoms in the direction of longitudinal axis of tube; 3) Transverse phonon modes that model vibrations of carbon atoms perpendicular to the longitudinal axis of the tube. Although, both transverse and longitudinal phonon modes have two optical and acoustical branches, the RBM phonon mode is just optical. Raman scattering spectra show three peaks in the energy, the G-band, D-band, and radial breathing mode (RBM) which can be used as the distinctive characteristic of SWCNTs.\textsuperscript{23} RBM peaks, which appear in the lower frequency region ($<400\, \text{cm}^{-1}$), are used to establish the tube diameter ($d$) and chirality ($n_1, n_2$) analysis based on the resonant Raman scattering effects\textsuperscript{24,25}. Then RBM describes nanotube uniquely\textsuperscript{26} and it is used for characterization of the nanotube in laboratory\textsuperscript{27}. Phonons affect strongly CNTs conductance, and e–ph coupling plays a crucial part in the perception of properties of CNTs. In low-bias regime, because of electron-acoustic phonon interactions weakness, it is observed that, ballistic conductance occurs.\textsuperscript{28–30} In high-bias regime, high-energy vibrational modes are excited and interaction between electrons and these phonons restricts ballistic conductance\textsuperscript{31}. e–ph interaction in metallic CNTs has a strong effect on the current behavior in different temperatures\textsuperscript{32}. In this paper, we study the effect of electron–RBM phonon interaction in metallic zigzag CNT on variations of current by using energy analysis approach. It has been observed that due to the electron–RBM phonon interaction, the current changes in a step–like form as a function of bias voltage. It means that creating a new phonon mode, in addition to the others, gives rise to changing the current for certain values of energy changing. Temperature is a significant parameter in the conductance of CNTs\textsuperscript{33} as our results have demonstrated that in low temperature and bias voltage, e–ph interaction is not an important factor in current changes; but in higher temperatures because of excitation of high energy optical phonon modes, the e–ph interaction has more important effect on the decreasing of the current.
The arrangement of this paper is as follows. First, in section II A, the electron dispersion relation for zigzag CNTs is presented. In Sec. II B, we present both approximations of the RBM frequency as well as Fröhlich Hamiltonian to describe the e–ph coupling with the corresponding coefficient for this type of atom vibrations. Further, to tackle the signature of interaction between the electron and RBM phonon on the correction of the current, we consider a CNT coupled to two reservoirs and apply energy analysis method in Sec. II C. We focus on the obtained results in the Sec. III, and describe how the temperature and the voltage affect the current. Finally, the paper is briefly concluded and summarized in Sec. IV.

II. THEORY

A. Electronic structure of CNTs

The structure of a SWCNT is uniquely defined by the chiral vector $C$ which indicates the rolling up direction. Since CNT is a cylindrically rolled counterpart of a graphene sheet, $C$ in terms of unit vectors of graphene, is expressed as, $C = n_1 a_1 + n_2 a_2$ in which $a_1$ and $a_2$ are chiral indexes. Besides, to calculate the electron dispersion relation of zigzag CNTs, we apply zone-folding method\(^{34}\) on the relation derived by the tight binding model of graphene under nearest neighbor approximation\(^{17}\) for $\pi$-electrons. In this method, by using periodic boundary conditions in the circumferenceal direction denoted by the chiral vector $C$, the wave vector associated with the $C$ direction becomes quantized. Thus, the energy bands consist of a set of one-dimensional energy dispersion relations. Assuming the vanishing orbital overlap, electron dispersion relation of $(n,0)$ zigzag CNTs would be

$$E^\pm_{\pi}(m,k_z) = \gamma_0 \sqrt{3 + 2 \cos(\frac{2\pi m}{n}) + 4 \cos(\frac{\pi m}{n}) \cos(\pi k_z)}.$$  (1)

Here, $\gamma_0 \approx 3.033$eV, is the nearest neighbor hopping energy, $k_z$ shows the component of the wave vector parallel to the CNT’s axis where $m$ and $n$ satisfy $-(n-1) \leq m \leq n$. For a general $(n,0)$ zigzag carbon nanotubes, when $n$ is a multiple of 3, the energy gap becomes zero at $k = 0$ and CNTs show metallic behavior.

B. Coupling between electron and Radial-breathing mode phonon

$e$–$\phi$ interaction has a key role in the perception of electronic, optical and transport properties of CNTs\(^{30}\). To address CNTs identification in particular of their chirality, we study the effect of radial-breathing mode of phonons on CNTs conductance. Coherent vibrations of carbon atoms in the direction of nanotube diameter result in RBM phonons and their frequency depends on the inverse of CNTs diameter\(^{23,27,35}\). In this paper we considered two approximations for the frequency of RBM mode. In the first one, the frequency of RBM phonons can be achieved from the continuum mechanics of a small hollow cylinder shown by Mahan\(^{36,37}\) as

$$\omega_{\text{RBM}} = \frac{c_1}{d} + \frac{c_2}{d^3},$$  (2)

where for an isolated nanotube, theoretical and experimental reported values of constant coefficients are $c_1 = 218$ to $248 \text{ cm}^{-1} \text{nm}$ and $c_2 = 0.17^{,38}$. By adopting the approximation used in Ref.\(^{37}\), for metallic CNTs, we consider $c_1 = 243 \text{ cm}^{-1} \text{nm}$ and $c_2 = 0$. For small diameter CNTs, a more precise approximation can be used as a tensional force results in distortion of its band structure\(^{39}\). The $\omega_{\text{RBM}}$ in this approximation (the second approximation) would read as

$$\omega_{\text{RBM}} = \frac{c_1}{d} + \frac{c_2}{d^3},$$  (3)

where $c_1 = 226 \text{ cm}^{-1} \text{nm}$ and $c_2 = 1.5 \pm 0.5 \text{ cm}^{-1} \text{nm}\(^{37}\)$. For small diameter nanotubes, effects of rolling nanotubes cause noticeable deviation from the simple appropriation of $\omega_{\text{RBM}}$ with the inverse of CNT diameter. In order to model the e–$\phi$ interaction, Fröhlich proposed the below Hamiltonian which is especially suitable for transport. Assuming that e–$\phi$ coupling occurs with the same coefficient, the e–$\phi$ interaction Hamiltonian can be written as

$$H_{e-\phi} = \sum_{k,k'} M_{k,k'} (c_k^\dagger c_{k'}) (a^\dagger_a + a_q) c_{k'}^\dagger c_{k'},$$  (4)

where $c_k^\dagger$ and $c_{k'}$ ($a^\dagger_a$ and $a_q$) are Fermionic (Bosonic) creation and annihilation operators respectively, $M_{k,k'}$ shows e–$\phi$ coupling coefficient and sum is over all electronic states. The diagonal matrix elements of the e–$\phi$ coupling Hamiltonian for optical phonons can be obtained from the shift of the electronic bands under deformation of the atomic structure corresponding to the phonon–pattern\(^{37}\)

$$M_{e-\phi} = \frac{\hbar}{2m N \omega_{\text{RBM}}} \sum_a E_a \frac{\partial E_b(k)}{\partial u_a},$$  (5)

in which $m$ is the atomic mass of electron, $N$ represents the number of unit cells and $a$ indexes the atoms in the unit cell of the nanotube. $E_a$ refers to the normalized phonon eigenvector and $\frac{\partial E_b(k)}{\partial u_a}$ describes the changes in the electronic energy $E_b$ due to the atomic displacement $u_a$. Because $\frac{\partial E_b(k)}{\partial u_a}$ is proportional to $d^{-141}$, $M_{k,k'}$ can be written as

$$M_{k,k'} = \frac{1}{d} \sqrt{\frac{\hbar}{2m N \omega_{\text{RBM}}}}.$$  (6)

C. Conductance calculation

Now consider a bias voltage $eV << E_F$, where $E_F$ is the Fermi energy of electrons in the nanotube, applied on the mesoscopic structure including a metallic zigzag SWCNT, which its length is much larger than its diameter and it is connected to metallic reservoirs. It is assumed that the length of
two metallic electrodes is in the order of $A_F$, hence, the trans-
portation of ballistic electrons through the nanotube is robust
against the edge effect. In addition, the rate reduction of the el-

cetric field in the nanotube is proportional to $a/L$ (where $1.25 < a < 1.75 \text{ Å}$ and $L$ is the nanotube length). The con-
duction of the nanotube can be divided into two main parts: edge and central parts. Also, it has been assumed that the
electron and phonon population is in balance and they behave independently. Thus, the e–ph interaction can be considered
as a perturbative phenomenon. In the following, we investig-
ate the influence of e–ph coupling on the changes of current
in the central part of a nanotube.

The total Hamiltonian of the system can be described by

$$H = H_0 + H_1 + H_{e-ph},$$

where, the kinetic energy ($H_0$), the interaction between elec-

trons and electrical field ($H_1$), and the e–ph coupling in the
elastic regime ($H_{e-ph}$) are respectively given by

$$H_0 = \sum_k \epsilon c_k^{\dagger} c_k + \sum_q \hbar \omega_q a_q^{\dagger} a_q,$$

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

$$H_{int} = \sum_{k,k'} M_{k,k'}^{q} (a_{-q}^{\dagger} + a_{q}^{\dagger}) c_{k}^{\dagger} c_{k'},$$

where $v_z$ is the electron velocity along the nanotube. Ac-

cording to the elasticity of e-ph scattering, only the interac-
tion of electrons with electronic field gives rise to energy loss.

Then, the change in the electron current is related to the rate of energy dissipation by

$$\Delta I = \frac{dE}{dt} = \frac{d}{dt} < H_1 >,$$

where

$$< O >= \frac{1}{i\hbar} < [H_1, H_{int}] >,$$

and all operators are in the Dirac representation. The statistical
operator $\rho(t)$ comply with equation

$$i\hbar \frac{d\rho}{dt} = [H_{int}(t), \rho(t)],$$

where $\rho$ is the density operator of electrons. The change in the
electronic current due to the electron-phonon coupling can be determined using the perturbation theory,

$$\Delta I = \frac{1}{i\hbar V} \text{Tr} \left[ \rho_0 [H_1, H_{e-ph}] \right],$$

the first order of the current variation is always equal to zero.
The first non-zero term is equal to

$$\Delta I_1 = -\frac{1}{\hbar^2 V} \int_{-\infty}^{t} dt' \text{Tr} \left[ [H_1, \rho] [H_1, H_{e-ph}] \right].$$

Consequently, by means of Wick’s theorem, we reach the first-
order correction on ballistic current, as

$$\Delta I = \frac{-e}{\hbar^2} \sum_{k,k',q} \text{sign}(v_z) \left( \text{sign}(v_{z'}) - \text{sign}(v_{z''}) \right) \delta(\epsilon_{k'} - \epsilon_k - \hbar \omega_q)$$

$$|M_{k,k'}^{q}|^2 \left[ N_q (f_k - f_{k'}) + f_k (1 - f_{k'}) \right],$$

Here $v_z$, the parameter of sign function, shows the speed of
electron and determines the direction of electron motion. $\epsilon_{k,k'}$ refers to the electron energy, $\omega_q$ shows the phonon
frequency, $M_{k,k'}^{q}$ is the e–ph coupling coefficient, $N_q$ and $f_{\alpha\beta}$
denote Bose–Einstein and Fermi–Dirac statistical functions,
respectively. At room temperature, the Fermi–Dirac distribu-
tion function behaves as a step function. The Fermi energy
of CNT electrons is roughly 2.9 eV and the Fermi level has
been considered as the reference of energy and sets to zero.

Under the first order of tight–binding method and Einstein
approximation, correction on the current is given by

$$\Delta I = \frac{-e\omega_0}{2M_N \hbar t} \sum_{k,k'}$$

$$\int_{-\infty}^{t} \int_{-\infty}^{t} dk'_c dk'_D \left( \text{sign}(v_{z'}) - \text{sign}(v_{z''}) \right) \delta(\epsilon_{k'} - \epsilon_k - \hbar \omega_q)$$

$$\left[ \frac{1}{\epsilon_{k}(\epsilon_{k} + \omega_0)} \right] \left( \theta(\frac{eV}{2} \text{sign}(v_{z'} - \epsilon_k)) - \theta(\frac{eV}{2} \text{sign}(v_{z'} - \epsilon_k') - \theta(\frac{eV}{2} \text{sign}(v_{z'} - \epsilon_k')) \right),$$

in which $q$ represents the branch of RBM and quantities of $k_z, k'_z$ are taken from quantization condition for nanotube.

Moreover, $D = \frac{a_0}{d}$ and $\frac{a_0}{\sqrt{(c_d + c_d')}}$ in the first and second approx-
imation of $\omega_{RBM}$, respectively. The first term indicates
interaction with thermal phonons which change the moment-
num of the electron. Besides, at very low temperatures, the

FIG. 1: (Color online) proposed mesoscopic system. SWCNT is
smoothly connected two massive metallic bulk reservoirs. The con-
ductance of this system is divided two parts: end parts and central
part.
second term is not zero because electrons gain energy due to applying electrical field and are able to transfer from a full level to an empty one by absorbing phonon, or transfer to a lower energy level and give their energy to the lattice by emitting phonon.

### III. RESULTS AND DISCUSSION

In this section, we present our results for the changes in the conductance due to the e-ph coupling, as a function of the bias voltage and temperature. Moreover, the results of different CNT diameter size and different $\omega_{RBM}$ frequencies are compared. Electrical current correction diagram of metallic zigzag CNTs as a function of Voltage has been represented in Fig.(2), for different diameters in the presence of e-ph interaction in RBM. Electrons move along nanotubes affected by the bias voltage. When the voltage increases, electrons gain sufficient energy for interaction with phonons. Interaction occurs for given quantities, because of quantization of phonons energy, and the electrical current increases step–likely. At room temperature, high energy RBM phonons do not exist, so scattering from optical phonons contains phonon emission. Also step–like changes of current for smaller diameter nanotubes are greater because e-ph interaction decreases by increases of nanotube diameter. In small diameter nanotubes, electrons are not able to move from bonds that do not cross the Fermi level.

![Fig. 2: (Color online) Electrical current correction diagram as a function of voltage for three different metallic zigzag CNTs by considering e-ph interaction in RBM.](image1)

Fig.(3) represents diagram of current correction as a function of voltage considering electron-RBM phonon for (9,0) zigzag CNT in three different temperatures. At temperatures that are lower than room temperature, thermal phonons contribution is small and excited phonons have a little effect on current changes. When temperature increases, approaching room temperature, the energy of excited modes increases and e–ph scattering has more contribution in the current decrease.

![Fig. 3: (Colour online) Electrical current correction diagram as a function of voltage by considering electron-RBM phonon coupling for (9,0) zigzag CNT in three different temperatures.](image2)

The second approximation has been used for $\omega_{RBM}$ due to considering distortions of the band to calculate the variations of the current and has compared with results of first approximation for $\omega_{RBM}$ in Fig.(5) (a) and (b). This figure represents variations of the current versus the bias voltage considering electron-RBM phonon interaction in (6,0) zigzag nanotube by second and first approximations for $\omega_{RBM}$ and Fig.(5) (c) and

![Fig. 4: (Color online) The current variation as a function of temperature, considering e-ph interaction in two different constant voltages.](image3)
of current variations in small diameter nanotubes, is noticeably more than large diameter nanotubes. In other words, the decrease in the difference between results of two approximations is related to decrease of e-ph interaction in larger diameter nanotubes which causes effects of nanotubes diameter to weaken in current variations.

IV. CONCLUSION

In conclusion, we demonstrated that, as the bias voltage increases sufficiently, the creation of a phonon gives rise to specific current variations which directly depends on the diameter. Current variations, based on the electron-RBM phonon coupling, are step-like function of bias voltage. Besides, one can observe that current variations increase by decreasing the diameter of nanotube since electron-RBM phonon coupling reduces as the diameter of nanotube rises because in this case CNTs behave as same as graphene sheet and the electron-RBM phonon interaction can be neglected. Moreover, as infinite CNTs has the continuous energy spectrum along its axis direction, when the energy is induced into the system, at the first, low energy phonons are created and following the continuous energy increase, higher energy phonons emerge. To shed light on the study of CNTs properties, we proposed a simple method for creation and characterization of RBM phonons of metallic zigzag nanotubes by electron injection. As in experimental realization, a branch of CNTs with different shapes and sizes are produced, it is essential to characterize their diameter. Since RBM mode determines the geometry and structure of CNT, by following the peaks of the conductance we can trace the different CNTs in a sample. So this approach can be a proper and simple method for the identification of CNTs.

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