Effects of electron-phonon interaction on transport through carbon nanotubes: lifting of degeneracies in Fock-space

Luis E F Foa Torres 1,2 and Stephan Roche 2

1 CEA Léti - MINATEC, CEA-LETI, MINATEC, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France.
2 CEA/DSM/DRFMC/SPSMS/GT, 17 avenue des Martyrs, 38054 Grenoble Cedex 9, France

Abstract. In this contribution we present a brief overview of recent results about the effects of electron-phonon interaction in electronic transport through metallic single-walled carbon nanotubes. In particular, we present an electron-phonon-induced backscattering mechanism which can be seen as the removal of degeneracies in the electron-phonon Fock space. This mechanism, which is activated when driving the system out of equilibrium, is beyond the scope of commonly used mean field approaches. Possible experimental consequences of such phenomenon are also discussed.

1. Introduction
Since their discovery, carbon nanotubes (CNTs) have attracted much attention due to their outstanding mechanical and electrical properties [1, 2]. They present an anomalously low sensitivity to disorder-induced backscattering [3] and unique spectral features [4]. Besides, despite of being quasi one-dimensional materials, the Peierls instability is inefficient to open a significant energy gap [5] except at very low temperatures (∼10K) [6] or for very short radius tubes (∼0.2nm) [7]. The existence of semiconducting nanotubes results from well-defined helical symmetry dependent selection rules that forbid the existence of eigenstates at the Fermi level. Technological interest is driven by applications such as nanotube-based field effect transistors, interconnects and memories.

Transport experiments on metallic tubes with low resistance contacts show two different regimes: the low and the high bias regimes. At low bias voltages, experiments performed on clean samples using low resistance contacts demonstrate a regime of almost perfect ballistic transport for tube lengths of up to ∼ 500nm [8, 9]. In contrast, at high bias voltage V (> 0.2 V) the resistance rapidly increases leading to current saturation for tubes of lengths L > 300nm [10, 11, 9], a behavior which has been attributed to electron-phonon (e-ph) interaction [10] with optical phonons.

These experimental results triggered several theoretical studies [12, 13, 14] (see also [15] and references therein). The approaches that were used include simulations based on the Boltzmann equation, the Fermi golden rule, the Kubo approach and the self-consistent Born approximation. Besides, in order to explain the quantitative disagreement between theoretical and experimental estimations of inelastic mean free paths, a hot phonons scenario was proposed [13]. Calculations based on the Fermi golden rule as well as the Boltzmann equation for the coupled electronic and
phonon dynamics indicate an onset of a high nonequilibrium optical phonon occupation (hot phonons) at high bias. The phonon occupations obtained in Ref. [13] are in the order of 3-5.

On the other hand, electron-phonon interactions in these low-dimensional systems can lead to more subtle effects introducing important corrections to both phonon and electronic band structures. Fundamental examples are the Kohn anomaly [16, 17], the anomalous behavior of the phonon dispersion due to electronic screening of vibrations, and the Peierls instability [18, 5]. Similarly, the activation of vibrational modes has also some direct influence on the of the phonon dispersion due to electronic screening of vibrations, and the Peierls instability structures. Fundamental examples are the Kohn anomaly [16, 17], the anomalous behavior to more subtle effects introducing important corrections to both phonon and electronic band

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proposed in Ref. [20] and further develop on possible experimental consequences that can be overview of these recent results is presented. Specifically, we will briefly introduce a mechanism proposed in Ref. [20] and further develop on possible experimental consequences that can be foreseen based on a simplified analysis.

2. Results and Discussion

Among the optical phonon modes that produce a strong coupling with electrons in the neighborhood of the charge neutrality point (CNP), only the Γ point \( A_1(L) \) mode are considered. The associated lattice displacements for a zig-zag tube are shown schematically in Fig. 1-a, A-type and B-type atoms move out of phase generating a dynamical Peierls-like distortion. To obtain a grasp of the effect of this distortion, we consider a simple Hamiltonian model. Let us assume a Hamiltonian that is the sum of an electronic part, a phonon part and an electron-phonon interaction term, \( H = H_e + H_{ph} + H_{e-ph} \). The electronic part is described through a \( \pi \)-orbitals effective model (i.e. a single \( \pi \) orbital per carbon atom) [1]:

\[
H_e = \sum_i E_i c_i^+ c_i - \gamma_0 \sum_{\langle i,j \rangle} [c_i^+ c_j^+ + H.c.],
\]

where \( c_i^+ \) and \( c_i \) are the creation and annihilation operators for electrons at site \( i \), \( \gamma_0 \) is the \( \pi-\pi \) integral overlap, the second summation is restricted to nearest neighbors in the tube. Now, we consider the effect of e-ph interaction with the \( A_1(L) \) phonons. This will introduce an e-ph interaction term \( H_{e-ph} \) which leads to a phonon induced modulation of the electronic coupling terms [21], by keeping only the linear corrections to the atomic displacements from equilibrium one gets an interaction term of the form:

\[
H_{e-ph} = \sum_{\langle i,j \rangle} \left( \gamma_i^{e-ph} c_i^+ c_j + b_{A_1(L)}^+ + b_{A_1(L)} \right) + h.c.,
\]

where \( b_{A_1(L)}^+ \) and \( b_{A_1(L)} \) are the phonon operators.

For the case of zig-zag tubes, the electronic properties close to the CNP can be described by two independent propagating channels. Furthermore, due to the symmetry of this phonon mode, e-ph interaction does not mix them. The dispersion relation \( \varepsilon^{(0)}(k, n) \equiv \langle k, n | H_e + H_{ph} | k, n \rangle \) for one of those channels is shown in Fig. 1-b, different curves correspond to different values of the phonon occupation \( n \), \( k \) is the electronic quasi-momentum in the direction parallel to the tube axis. The crossing points between these curves correspond to degenerate states in the e-ph Fock space differing in one phonon. These states are mixed by the e-ph interaction term thereby removing their degeneracy [20] and opening energy gaps at half the phonon energy, \( \hbar \omega_0/2 \), above (below) the CNP associated to phonon emission (absorption). The resulting e-ph
induced energy gaps can be estimated from the precise form of the e-ph matrix elements [20] and assuming a thermalized phonon occupation, the resulting values are in the order of 32 meV. It should be noted however that this mechanism cannot be activated unless the system is driven out of equilibrium. This is because Pauli Blocking forbids strong inelastic processes when the system is close to equilibrium, a restriction that can be overcome by applying a high enough bias voltage ($eV \sim \hbar \omega_0$).

Figure 1. a) Representation of the atomic displacements induced by $Γ$ point $A_1(L)$ phonons in a zig-zag tube. b) Scheme for the unperturbed ($H_{e-ph} = 0$) dispersion relations for an electronic propagating channel close to the CNP. At the crossing points between these curves (see right panel), the e-ph interaction can lift the degeneracies leading to the opening of energy gaps. c) Numerical results for the transmission probability in the presence of e-ph interaction. Notice the gap that develops as the tube length $L$ increases. d) Current-voltage characteristics for a 100nm long tube contacted between metallic electrodes and including the e-ph interaction with $A_1(L)$ phonons.

Numerical results for the one particle transmission probability (including elastic and inelastic processes) for a tube of length $L$ contacted between metallic electrodes are shown in Fig. 1-c. There one can notice the appearance of a gap at energies around half the phonon energy above the CNP which progressively deepens as the tube length increases, being fully developed for $L \sim 100\text{nm}$. Results for the low temperature current-voltage characteristics for a tube of 100 nm length are shown in Fig. 1-d. There we can see that, although there is no influence on the low bias properties, the proposed mechanism would manifest as a plateau at $eV \sim \hbar \omega_0$ due to strong inelastic backscattering. Figure 1-c and d correspond to a thermalized phonon occupation ($n = 0$). Increasing the phonon occupation leads to a broadening of the gap and of the plateau observed in the I-V curve.
3. Conclusions

Two key ingredients for the proposed mechanism should be emphasized. The first is the dimensionality of the system, as in the case of the Peierls transition [18, 22], it is the dimensionality that allows for a single lattice oscillation to open an energy gap. On the other hand, since the considered phonon mode does not freeze in the considered temperature range, the equilibrium position of the atoms remain unchanged while they swing back and forth. This requires to go beyond the adiabatic approximation and the resulting non-equilibrium gap opens at $\hbar \omega_0/2$ above the CNP (Note that the adiabatic approximation would lead to a gap at the CNP instead [19]). Similar phenomena, although predicted within the adiabatic approximation, were recently reported [23].

Finally, we note that phonon modes other than the one considered here could lead to the same phenomenon if they produce a distortion of appropriate period in the axis direction. Further work along this line is in progress and many other interesting issues remain open, such as the effect of gating and/or doping of the nanotubes.

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