The influence of electro-mechanical effects on resonant electron tunneling through small carbon nano-peapods

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**Abstract.** The influence of a fullerene molecule trapped inside a single-wall carbon nanotube on resonant electron transport at low temperatures and strong polaronic coupling is theoretically discussed. Strong peak-to-peak fluctuations and anomalous temperature behavior of conductance amplitudes are predicted and investigated. The influence of the chiral properties of carbon nanotubes on transport is also studied.
1. Introduction

Carbon nano-peapods were discovered almost one decade ago [1] (see also the review papers [2]–[4]). They have been proven to be novel graphitic structures with electrical and mechanical properties that cannot be reduced to the sum of properties of their subcomponents (an empty carbon nanotube and individual fullerene molecules). Peapods, a composite system consisting of a rigid single-wall nanotube (SWNT) cage and an inner mechanically soft chain of fullerenes, can exhibit interesting nano-electro-mechanical properties if the coupling of delocalized electron states on the tube with the fullerene molecular orbitals is sufficiently strong. Buckyballs inside a SWNT are neutral objects and one cannot expect any direct electrical influence of encapsulated molecules on electron transport along a nanotube shell. However, STM spectroscopy of semiconducting peapods [5] showed that the local electron density of states (DoS) in carbon nanotubes is strongly modified by encapsulated C\textsubscript{60} molecules. These measurements can be theoretically interpreted in terms of a strong hybridization of electronic states on the nanotube surface with the lowest unoccupied molecular orbitals (LUMO) of the encaged C\textsubscript{60}. The corresponding hybridization strength was estimated in [5, 6] to be close to 1 eV. This energy is comparable to other characteristic energies of SWNTs and this means that virtual hopping of delocalized electrons from the SWNT to the local LUMO states is possible and can strongly influence the electronic properties of the SWNTs. Even though all samples in the cited experiment were semiconducting nanotubes, one could expect from theoretical considerations an analogous strong hybridization at least for chiral metallic nanotubes (see [6] where a theory of scanning tunneling spectroscopy of long C\textsubscript{60} peapods was developed). Notice that such a strong hybridization between fullerene- and nanotube-derived energy levels in peapods could shift the LUMO states even below the Fermi energy of the SWNT. This possibility was however ruled out in recent photoemission experiments [7].

In this work, we suggest that a strong coupling between the electronic states on the SWNT shell and the localized states on the fullerenes affects resonant tunneling transport of electrons through the metallic peapod system in a manner that is experimentally observable. In particular, we propose that resonant electron transport due to polaronic effects provides a method for studying the fullerene nanomechanical dynamics through the temperature dependence of the resonant conductance peaks. This should be readily observable since the characteristic temperature scale for the strong polaronic modification of the peaks is set by the fullerene vibration frequencies and may be very low compared to typical electronic energies.
Recent experiments with high-quality peapods demonstrated Coulomb blockade and Kondo physics at low temperatures \[8, 9\]. The spacings of conductance peaks was found to be regular over a wide range of gate voltages, indicating that the constant interaction model of Coulomb blockade (see e.g. \[10\]) applies for these dots. The peak amplitudes, on the other hand, strongly fluctuate from peak to peak. In the case of an empty metallic SWNT both peak spacings and amplitudes should ideally vary slowly with the gate voltage, except for variations of level spacings dictated by the particular SWNT bandstructure which leads to four-electron shells. While earlier experiments on empty nanotubes have exhibited strongly fluctuating peak conductances (see e.g. \[11\]), defect-free SWNTs have indeed shown remarkably gate-independent peak amplitudes \[12, 13\].

We show here that for carbon nano-peapods, electro-mechanical effects can lead to strong fluctuations of the Coulomb peaks. The mechanism will be effective even with defect-free nanotube shells. This phenomenon may explain the strongly fluctuating peak amplitudes seen in peapod experiments \[8, 9\]—detailed studies of Coulomb blockade peak fluctuations could thus reveal polaronic effects in quantum dots (QDs). Molecular conductors constitute another important class for which the vibronic coupling is also nearly always present, and for which it plays a fundamental role in the study of the transport properties, see \[14, 15\] and references therein.

The paper is organized as follows. In the following section 2, we investigate how the presence of even one encapsulated fullerene molecule, treated as a short-range scattering potential, can influence the electron energy spectrum of the SWNT by a strong polaronic effect. This will allow us to define the Hamiltonian of the peapod in an independent electron model. In section 3, the current through the peapod and hence its conductance are evaluated and studied, in this regime of strong polaronic coupling. Since the fullerene scattering potential in reality has an intermediate range, we discuss in section 4 how the peapod conductance is affected in the opposite limit of a long-range fullerene-induced scattering potential. Here, the appropriate model for the SWNT electrons involves the use of the Dirac equation. Finally, in section 5 we present our conclusions.

2. Energy spectrum in the presence of a short-range scattering potential: the model

The position of an individual buckyball inside the tube, for a partially filled peapod, is not fixed, and mechanical motion of the fullerene is excited in the process of virtual electron transitions onto and off the fullerene LUMO level. The effective excitation energy \(\hbar \omega_0\) strongly depends on the buckyball confinement potential. For vibrations in the nearly harmonic (for small displacements) transverse Girifalco potential \[16, 17\] the corresponding energy \(\hbar \omega_t\) is of the order of milli-electron-volts. Notice that electro-mechanical vibrations of C\(_{60}\) in the van der Waals-like potential between two gold electrodes have already been measured (\(\hbar \omega_0 \approx 5\) meV) in tunneling experiments \[18\]. The longitudinal motion of C\(_{60}\) inside the tube is less restricted and the corresponding excitation energy \(\hbar \omega_l\) could be much smaller. It is worth noticing here that the nanotube shell of peapods can in fact be quite full of large (~1 nm) holes in the tube walls. Only a small number of openings, used before to fill the tube, are healed in the post processing \[19\]. The average spacing between the holes can be estimated to be ~5–10 nm \[2\]. The holes produce a repulsive potential for fullerenes inside the tube, which we will model in our analytical calculations as a harmonic confinement potential.
potential with a characteristic energy $\hbar \omega_0 \sim 0.1$ meV, corresponding roughly to the zero-point energy of a C$_{60}$ confined to a length equal to the estimated average spacing between holes.

We start with a single encapsulated C$_{60}$ placed at a distance $l$ from the nanotube end. The virtual processes of electron hopping onto and off the fullerene LUMO level (shifted upwards by the charging energy $\sim e^2/2d$, where $d$ is the fullerene diameter) produce a local attractive potential for conduction electrons on the tube [6]. The first question one has to consider in order to formulate a theoretical model for the problem is whether this potential is short- or long-range with respect to its effect on electrons in metallic nanotubes. If the characteristic length of the scattering potential due to the fullerene is defined by its diameter, of the order of 1 nm, its range is determined by a comparison with the Fermi wavelength, $\lambda_F$, of electrons in a metallic SWNT. Since $\lambda_F \sim 7$ Å, [20], and hence is remarkably close to the fullerene diameter, the range of the potential is of intermediate range. It is therefore not a priori clear which of the two different limits, where an analytical investigation is possible, is the more appropriate one and we shall therefore discuss both.

In the first limit, the scattering potential is described as a short-range potential, which means that the hybridization-induced scattering potential is able to strongly backscatter electrons with a large momentum transfer, $\delta k \simeq 2k_F$. This is the regime studied in this section by means of a single-electron model. In the opposite limit the scattering potential is described as a long-range potential when the real band structure of the SWNT becomes important. This limit is hence discussed in section 4 using the Dirac equation.

A short-range hybridization-induced scattering potential with the hybridization strength $t_h \simeq 1$ eV changes the distribution of level spacings in the conduction band of a finite-sized nanotube. By solving the Schrödinger equation on a finite interval ($L$) with a $\delta$-function scatterer placed at point $x = l$ one gets the spectrum equation

$$k \sin k L = U(k) \sin kl \sin (k(L - l)), \quad (1)$$

where $k$ is the electron wavevector, ($\epsilon = \hbar^2 k^2/2m$), and the amplitude of the local scattering potential in our case represents the hybridization potential of [6]. In our notation

$$U(k) = \left(\frac{k_F^2}{\epsilon_F}\right) V_h(\epsilon), \quad V_h(\epsilon) = \frac{|t_h|^2 d}{E_0 - \epsilon}. \quad (2)$$

Here, $d \simeq \lambda_F$ and $E_0 > \epsilon$ is the energy of the hybridized side-level ($E_0 \simeq 2\epsilon_F$ if one takes into account the charging energy for electron hopping to the C$_{60}$ LUMO level).

The energy spectrum of equations (1) and (2) when $l/L$ is not a small rational number is irregular for energies not far from the Fermi energy (see figure 1), and indicates certain deviations from the mean level spacing $\Delta_L = \pi \hbar v_F/L$ (notice that due to the two identical conduction bands in a SWNT its mean level spacing is $\Delta_L/2$). However, as one can see from figure 1, for a single scatterer the ‘randomization’ is not pronounced even for energies close to the Fermi energy. About 40% of the levels deviate from the mean level spacing less than 18%, and among these levels 75% deviate less than 12%.

A shift $\delta x$ in the position of a scatterer leads to shifts of all quantized energy levels

$$\delta \epsilon_n = \hbar v_F \frac{\partial k_n}{\partial x} \delta x, \quad (3)$$

where the derivative of electron momentum with respect to scatterer position can easily be found from equation (1).
Figure 1. Energy levels, \( \varepsilon_n L/\hbar \nu_F \), for a peapod with just one fullerene inside. Unlike an empty SWNT, the spectrum is not uniform; still, for a single scatterer (fullerene), the randomization is not pronounced. The Fermi energy \( \varepsilon_F \) is such that \( \varepsilon_F L/\hbar \nu_F \sim 90 \).

In order to get analytical results we will model the potential that confines the longitudinal motion of our scatterer (buckyball inside a tube) as a harmonic potential. In the adiabatic limit, \( \omega_0 \ll \nu_F/L \), when the electron spectrum is well defined for any position of the vibrating impurity, the total Hamiltonian for a two-terminal conduction geometry reads\(^5\):

\[
\mathcal{H} = H_L + H_R + H_{T,L} + H_{T,R} + H_{QD},
\]

where \( H_\alpha = \sum_{k_\alpha} \epsilon_{k_\alpha} c_{k_\alpha}^\dagger c_{k_\alpha} \) is the Hamiltonian for the leads and \( \alpha = L, R \) for left and right reservoir, respectively. The QD Hamiltonian reads:

\[
H_{QD} = \sum_n \epsilon_n c_n^\dagger c_n + \sum_n V_n(L, l) c_n^\dagger c_n (b^\dagger + b) + \hbar \omega_0 b^\dagger b,
\]

where \( \epsilon_n \) is the set of levels shown in figure 1, \( \hbar \omega_0 \) is the vibration energy quantum, \( V_n(L, l) = \hbar \nu_F x_0 (\partial k_n / \partial l) \) and \( x_0 \) is the amplitude of zero-point fluctuations of the bosonic field \( (x_0 \approx 0.2 \text{ Å} \text{ for } C_{60} \text{ and for an energy value } \hbar \omega_0 \sim 0.1 \text{ meV}) \); \( c_n (c_n^\dagger) \) and \( b(b^\dagger) \) are fermionic and bosonic operators with canonical commutation relations. The tunneling Hamiltonian finally reads:

\[
H_{T,\alpha} = \sum_{k_\alpha, n} t(c_{k_\alpha}^\dagger c_n + \text{h.c.}),
\]

where we suppose that the hopping matrix elements \( t \) between the two leads and the dot are of the same order.

We should point out that the coupling to the electronic states of the SWNT does not significantly affect fullerene vibrations, which are mostly determined by fullerene confinement by structural defects on the carbon nanotube. This is true even though the coupling to each single electronic state may be strong and depend on the fullerene position. However, when evaluating the total fullerene energy shift caused by coupling to a very large number of different electronic

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\(^5\) The total Hamiltonian \( \mathcal{H} \) in equation (4) does not take into account the scattering potential represented by the holes on the tube shell. The possible consequences of such an issue are discussed in the conclusions.
states, the coordinate dependence averages out and such a coupling does not contribute to the mechanical force.

The Hamiltonian $H_{QD}$ can be diagonalized by means of a unitary transformation, see e.g. [21]: $\hat{H}_{QD} = e^S \hat{H}_{QD} e^{-S}$, with $S = \sum_n (V_n(L,l)/\hbar \omega_0) c_n^\dagger c_n (b^\dagger - b)$. The result of this transformation is

$$\hat{H}_{QD} = \sum_n (\varepsilon_n - \Delta) c_n^\dagger c_n + \hbar \omega_0 b^\dagger b,$$

where $\Delta = \lambda_n^2 \hbar \omega_0$ is the polaronic shift of the resonant energy level and $\lambda_n = V_n(L,l)/\hbar \omega_0$ is the electron–vibron coupling constant. The tunneling Hamiltonian is also transformed by the unitary transformation and it reads

$$\hat{H}_{T,\alpha} = \sum_{k_n,\alpha} t (c_{k_n}^\dagger c_n X + \text{h.c.}),$$

where the operator $X$ is defined as

$$X = \exp \left[ - \frac{V_n(L,l)}{\hbar \omega_0} (b^\dagger - b) \right].$$

3. Resonant tunneling

Resonant electron tunneling through a vibrating QD was considered in many papers (see e.g. [22, 23] and references therein). For a strong electron–phonon interaction, two non-perturbative effects determine the low-temperature electron transport—(i) a polaronic shift of the resonant energy level, $\varepsilon_n \to \varepsilon_n - \lambda_n^2 \hbar \omega_0$ and (ii) a ‘polaronic blockade’ (exponential suppression) of the peak conductance at low temperatures, $G_{\lambda_n} \propto \exp(-\lambda_n^2)$. In our case, the coupling ‘constant’ $\lambda_n$ is a level-dependent quantity and it strongly fluctuates from level to level. Such fluctuations are clearly visible in figure 2. We observe that these coupling constants being proportional to the derivative of the energy spectrum exhibit much more pronounced fluctuations than the energies themselves. The mean value of $\lambda_n^2$ for strong backscattering potential ($U(k_F) \sim \lambda_F^{-1}$) can be estimated as $\lambda_n^2 \sim (\varepsilon_F x_0/\hbar \omega_0 L)^2$. So, for the case of $N$ independent scatterers $N = L/d_c$, ($d_c$ is the characteristic range of the longitudinal confinement potential) the total polaronic shift will scale as $1/L$. Since the charging energy of our one-dimensional (1D) system also scales as $1/L$, it will be difficult to single out polaronic effects in the distribution of peak spacings as a function of gate voltage. Besides, the irregular character of level spacings could be caused by different physical effects, e.g. by electron scattering due to imperfections (holes) of the nanotube surface. Is there another manifestation of low-energy electro-mechanical effects in resonant electron tunneling?

3.1. Electric current

In order to study the peak-to-peak fluctuations in the electrical conductance, we first recover in this section the electric current flowing through the system.

We start from the well-known Meir–Wingreen formula [25, 26],

$$I(V) = -\frac{2e}{h} \int d\varepsilon \left[ f_L(\varepsilon) - f_R(\varepsilon) \right] \text{Im} \{ \text{Tr} \Gamma G_{QD}^\text{ret}(\varepsilon) \},$$

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Figure 2. Behavior of the polaronic coupling constant $\lambda_2^n$ as a function of state index $n$. The coupling constant strongly fluctuates since it is proportional to the derivative of the energy spectrum. The corresponding value for the 8th level, of the order of unity, is off the scale. The Fermi level is between the 10th and the 11th levels. We stress that we do not intend to show the actual and absolute numerical values of the couplings $\lambda$. These ‘constants’ can be obtained by fitting the experimental data to theory, as in [24]. The figure only aims to illustrate the strong level-to-level fluctuations of the coupling constant. In the case of $N$ independent molecules in the peapod, the average value of the coupling constant can be $N$ times larger than the values shown in the plot. In particular, the values of the coupling constant $\lambda$ shown in the plot have been evaluated for a sample whose length is 10 nm, and with a LUMO energy and a hybridization energy of the same order as the Fermi energy. These are the same values used to evaluate the spectrum in figure 1.

where $f_{L/R}(\epsilon) = \left\{ \exp\left[ (\epsilon - \epsilon_F + eV/2)/k_BT \right] \right\}^{-1}$ are the Fermi functions for the left and right reservoirs, $G_{QD}^{\text{ret}}(\epsilon)$ is the retarded Green function of the dot and $\Gamma = \Gamma_L \Gamma_R / (\Gamma_L + \Gamma_R)$. $\Gamma_{L/R} = 2\pi i^2 \rho_{L/R}$ are the widths of the resonance due to tunneling from the left or right lead, and $\rho_{L/R}$ is the DoS in the reservoirs.

In order to evaluate the current in equation (10), one needs the Green function of the dot which takes into account, at least in principle, not only all the possible processes in the dot, as inelastic processes and multiple scattering processes, but also the effects of the vibrons on the reservoirs [23, 25]. To get analytical results, we will treat the leads, as in [23], as unaffected by the vibrons modes in the dot. Besides, we suppose that the bandwidth in the contacts is much larger than both the resonance width and the vibron energy quantum, that is, we will evaluate the electron part of Green function in the so-called wide-band limit [27].

Under such assumptions, the retarded single particle Green function can easily be evaluated, see also [21], and it reads

$$G_{QD}^{\text{ret}}(t) \approx -i\Theta(t) \exp\left[ -\frac{i}{\hbar} \left( \epsilon_n - \Delta - i\frac{\Gamma_L + \Gamma_R}{2} \right) t \right] \exp\left[ -\lambda^2 \left( 2n(\beta \hbar \omega_0) + 1 \right) \right]$$

$$\times \sum_{l=\pm \infty} I_{l} \left[ 2\lambda^2 \left[ n(\beta \hbar \omega_0) \right] \left( n(\beta \hbar \omega_0) + 1 \right) \right]^{1/2} \exp\left[ l\hbar \omega_0 \left( \frac{t}{\hbar} - \frac{\beta}{2} \right) \right], \quad (11)$$
where \( n(x) = (e^x - 1)^{-1} \) is the Bose distribution, \( \beta = 1/k_B T \), \( I_l \) is the modified Bessel function of the first kind, and for sake of simplicity, we have omitted the index \( n \) from the coupling constant \( \lambda \). Equation (11) can be easily Fourier transformed and the expression of the current written as in \([23]\)

\[
I(V) = \frac{e}{h} \int \text{d} \epsilon [f_L(\epsilon) - f_R(\epsilon)] e^{-\frac{\lambda^2}{2n(\beta h_0 \omega_0) + 1}}
\times \sum_{l=-\infty}^{\infty} I_l(2\lambda^2 [n(\beta h_0 \omega_0)(n(\beta h_0 \omega_0) + 1)]^{1/2}) e^{-\lambda h_0 \beta/2} T_{BW}(\epsilon, l),
\]

where

\[
T_{BW}(\epsilon, l) = \frac{\Gamma_L \Gamma_R}{(\epsilon + i\hbar \omega_0 + \Delta_{pol})^2 + ((\Gamma_L + \Gamma_R)/2)^2},
\]

with \( \Delta_{pol} = \Delta - \epsilon_n \).

### 3.2. Electric conductance

A simple expression of the conductance can be derived from equation (12) in the linear regime, \( eV \to 0 \), and weak coupling to the leads, \( \Gamma_L + \Gamma_R \ll \min[k_B T, \hbar \omega_0] \). In addition to the latter condition, in order to have polaronic states, it is necessary, physically that \( \Gamma \ll k_B T \ll \lambda^2 \hbar \omega_0 \) as well. These conditions state that the time spent by the electron in the dot must be larger than the characteristic time needed to form a polaron. Under these assumptions, the Lorentzian in equation (13) is just a \( \delta \)-function centered at \( \epsilon = \epsilon_n - \Delta - i\hbar \omega_0 \). Then, the integral in equation (12) can be easily evaluated and the current reads

\[
I(V) = 2\pi e^2 h^{-1} \int \frac{\Gamma}{\epsilon_n - \Delta - i\hbar \omega_0 - f_L(\epsilon_n - \Delta - i\hbar \omega_0) - f_R(\epsilon_n - \Delta - i\hbar \omega_0)} e^{-\lambda^2 [2n(\beta h_0 \omega_0) + 1]} \cdot \frac{\lambda h_0 \beta}{2}.
\]

Since we are interested in the conductance peak height, we consider the physical condition where, by means of the gate voltage, the levels in the dot are tuned such that \( \epsilon_F = \epsilon_n - \Delta \). Then, in the limit \( eV \to 0 \), a simple analytical expression can be written:

\[
G_\lambda(T) = G_{\lambda=0}(T) F_\lambda(\hbar \omega_0/k_B T),
\]

where \( G_{\lambda=0}(T) \simeq (\pi/2)G_0 \Gamma/k_B T \) is the standard resonance conductance of a single-level QD \( (G_0 = e^2/h \) is the conductance quantum) and the function \( F_\lambda(x) \), with \( x = \hbar \omega_0/k_B T \), is represented as a series

\[
F_\lambda(x) = \exp\{-\lambda^2[1 + 2n(x)]\} \sum_{l=-\infty}^{\infty} \exp(-lx/2) I_l[2\lambda^2 \sqrt{n(x)(1 + n(x))}]/\cosh^2(lx/2).
\]

It is easy to check that \( F_{\lambda=0}(x) = 1 \).

For a strong electron–vibron coupling \( (\lambda \geq 1) \), polaronic effects can significantly suppress the conductance at low temperatures, \( (\Gamma \ll k_B T \ll h \omega_0) \), for which one finds \( F(x) \simeq \exp(-\lambda^2) \).

In this regime, the usual \( \sim 1/T \) behavior is recovered for the conductance, but the latter is strongly suppressed because of the factor \( \exp(-\lambda^2) \). This is the signal of the reduced probability for an electron to tunnel from a bare electronic state in the reservoir to a polaronic state.
Figure 3. Behavior of the conductance $\tilde{G}_{\lambda}(T) = \tilde{G}_{\lambda}\hbar\omega_0/T$ as a function of the renormalized temperature $\tilde{T} = k_B T/\hbar\omega_0$ and for three different values of the coupling constant $\lambda$. An anomalous temperature dependence of the resonance peak height is well visible in the region $k_B T \lesssim \lambda^2 \hbar\omega_0$. Inset: the behavior of the conductance for strong coupling, $\lambda = 3$, is shown in a narrow region close to zero temperature. The behavior is dominated by $\exp(-\lambda^2)/T$ close to zero. Then, the dominant term is proportional to $\sim (1/\sqrt{T}) \exp(-\lambda^2 \hbar\omega_0 / 4 k_B T)$.

The latter equation indicates that for temperatures larger than $\hbar\omega_0$, a competition arises between the vibrons and the polarons, giving rise to a non-monotonic behavior. At temperatures $k_B T \gg \lambda^2 \hbar\omega_0$, when the polaronic blockade is completely lifted, the conductance scales as $1/T$, as can be numerically verified. At such high temperatures, the polaronic effects get completely destroyed by the thermally excited vibrons. The temperature lifting of the polaronic blockade results in a non-monotonic temperature dependence of the conductance peak. This behavior is shown in figure 3, where we plot the temperature dependence of the amplitude of the Coulomb blockade conductance peak for different values of the electron–vibron coupling $\lambda$. It is clearly seen from the figure that polaronic effects are pronounced only for strong electron–vibron interaction ($\lambda \gtrsim 1$), and in the temperature region $k_B T \lesssim \lambda^2 \hbar\omega_0$ anomalous temperature dependence of resonance peaks appears. The observation in an experiment of a low-temperature scaling which differs from the usual $1/T$-dependence for narrow Coulomb blockade conductance peaks, in general, indicates that the level width is not the only relevant state in the dot. As soon as the temperature becomes of the order of $\hbar\omega_0$, thermally excited vibronic modes of the fullerene molecule appear. The characteristic energy of fullerene thermal vibrations is $n(\beta \hbar\omega_0)\hbar\omega_0$, $n(x)$ being the Bose distribution. This energy should be compared with the polaronic energy shift $\lambda^2 \hbar\omega_0$ induced by fullerene displacement. The corresponding ratio determines the relative strength of destructive influence of thermal vibrations on polaronic effects. Indeed, at temperatures $\hbar\omega_0 \ll k_B T \lesssim \lambda^2 \hbar\omega_0$, by keeping the first $l$-independent term in the asymptotic expansion of the Bessel function $I_l$, $F(x) \simeq ((\sqrt{\pi}/x)/\lambda) \exp(-\lambda^2 x/4)$, and the conductance reads,

$$G_{\lambda}(T) \simeq G_0 \frac{\Gamma}{\lambda\hbar\omega_0} \left( \frac{k_B T}{\hbar\omega_0} \right)^{-1/2} \exp\left( -\lambda^2 \frac{\hbar\omega_0}{4 k_B T} \right).$$  \hspace{1cm} (17)
energy scale in the problem. An anomalous temperature behavior and $1/\sqrt{T}$-scaling is the signature of strong polaronic effects, as experimentally observed [24].

4. Polaronic effects in long-range scattering limit

The polaronic effects discussed in the previous sections appear due to strong backscattering of the SWNT electrons by the fullerene-induced potential, which was assumed to be short-range. Here, we want to consider the opposite limit of a long-range potential, where we can also obtain an analytical solution. In this case, the real band structure of the SWNT electrons must be considered. It is known that the specific band structure (Dirac-like spectrum) leads to a new type of backscattering by even a long-range potential. In this section, we will study the influence on polaronic effects of this type of backscattering, which is closely related to the chiral properties of the carbon nanotube (the chiral angle).

The band structure of graphene in the vicinity of the Fermi energy (these points in the Brillouin zone of 2D graphite are usually labeled K and K’) is described by the Dirac Hamiltonian for massless fermions $H_D = \hbar v_F \bar{\sigma} \vec{p}$, [28] (see [29], where a Dirac-like energy spectrum in graphene was confirmed in experiments). Here, $\vec{p}$ is the 2D electron momentum, $\bar{\sigma}$ are the Pauli $2 \times 2$ matrices which describe the chiral properties (pseudospin) of particles and holes in each conduction band. The chiralities $\bar{\sigma} \vec{p} / |\vec{p}| = \pm 1$ of particles and holes are opposite in the same band and particles (holes) in different bands are characterized also by opposite chiralities. Conservation of chirality in scattering by a scalar potential leads to various unusual phenomena in graphene that are currently discussed in the literature (see, e.g. [30]). The wrapping of a graphene sheet into a SWNT results in a 1D relativistic form of the electron dispersion, which depends on the chiral indices of the nanotube, describes either massless (metallic SWNT) or massive (semiconducting SWNT) Dirac fermions $\varepsilon(q) = \pm \hbar v_F \sqrt{q^2 + \Delta_m^2}$, where $\Delta_m \propto 1/R_{NT}$ is the gap in electron spectrum, and $R_{NT}$ is the radius of the nanotube.

Now, we will treat the hybridization-induced scattering potential as a long-range potential [6] and reconsider the problem of resonant electron tunneling using the Dirac-like electron spectrum. Scattering of electrons by a long-range potential ($\delta k \ll k_F$) leaves the quasi-particles in the same band and thus does not mix particles (or holes) with opposite chiralities. In this case, the chiral properties of electrons in a SWNT play a significant role and should be taken into account. Using the same approach as in [6], we consider the spectrum problem for a short peapod and discuss possible polaronic effects in resonant electron transport through this system.

At the boundaries of a nanotube, $x = 0, L$, the scattering potential is sharp and this results in strong backscattering $\delta k \simeq 2k_F$ by the boundaries. The spinor wavefunction of an electron in a nanotube now takes the form $\Psi(x) = e^{ikFx} \Psi_+(x) + e^{-ikFx} \Psi_-(x)$, where subindices (+, −) label two identical bands of the energy spectrum. The general boundary condition for a finite-sized system of Dirac fermions is the absence of current through the boundaries. This condition is satisfied in our case if we assume perfect reflection at the boundaries, $L^\pm \leftrightarrow R^\mp$, where $R^\pm(L^\pm)$ denote right(left)-moving particles in the ‘+’ or ‘−’ band.

In [6], the scattering matrix for a long-range potential was calculated using the Dirac equation. Now, we would like to incorporate this result in order to consider resonant tunneling through the 1D wire. This can be easily done in the limit when the distances from the scatterer to the ends of the wire are much bigger than the spatial extension of the potential. Hence, if one is not interested in the exact position of the resonant level, then the resonant transmission
through the given level can be obtained in the approximation where the scatterer can be treated as a point-like defect. Such a defect will be characterized by the same scattering matrix obtained for the electrons propagating in an infinite wire as in [6].

The local (δ-function) potential at \( x = l \) now represents a long-range imperfection which scatters fermions only within its own band. The spectral problem can be solved by the standard method of finding the solution of the Dirac equation in the ranges \( x \neq l \) and matching them at \( x = l \) by using the properties of the Dirac equation in a δ-function potential. In the general case of massive Dirac particles, the spectrum equation is cumbersome and lengthy. We are interested in transport through a metallic SWNT, that is, in the case of a massless Dirac spectrum, \( \Delta_m = 0 \). In this limit, \( \epsilon = \pm \hbar v_F q \), the spectrum equation can be represented in the simple form

\[
 t(\theta, \phi) \cos(2k_F L) + r(\theta, \phi) \cos[2q(L - 2l)] - \cos(2q L - \phi) = 0, \tag{18}
\]

where \( t(\theta, \phi) \) and \( r(\theta, \phi) \) are the transmission and reflection coefficients for the δ-function potential scattering problem by massless chiral particles. In this case,

\[
 r(\theta, \phi) = \sin^2 \theta \sin^2 \frac{\phi}{2}, \tag{19}
\]

where \( \theta \) is the chiral angle of the nanotube and

\[
 \tan \varphi = \frac{2\hbar v_F V(\epsilon)}{(\hbar v_F)^2 - V^2(\epsilon)}, \quad V(\epsilon) = V_h(\epsilon). \tag{20}
\]

We see from equations (18)–(20) that for a massless Dirac spectrum the reflection coefficient vanishes for \( \theta = 0 \), that is, for armchair nanotubes. The corresponding spectrum is uniform with level spacing \( \pi \hbar v_F/2L \), and the total energy shift, \( \hbar v_F \varphi/2L \), is induced by forward electron scattering by the long-range potential. The absence of electron backscattering in non-chiral SWNTs (formally due to conservation of chirality) has repeatedly been discussed in the literature (see e.g. [30]). In general, the suppression of backscattering in metallic SWNTs as compared to semiconducting nanotubes (where the presence of a gap in the spectrum mixes states with opposite chiralities) is often used to explain the remarkably good conducting properties of long metallic carbon nanotubes [31].

For the spectrum in equation (18), one can easily estimate the electron–vibron coupling as \( \lambda \sim r(\theta, \phi)v_F x_0/\omega_0 L^2 \). Polaronic effects are determined by the square of this parameter, which is smaller by a factor \( (\lambda v_F/L)^2 \) than the analogous coupling expected for a short-range hybridization potential.

The origin of such a weak polaronic coupling constant resides in the strongly reduced backscattering processes, since polaronic effects are extremely sensitive to that. Then, in transport measurements, where electronic backscattering with a large momentum transfer is expected because of the same order of magnitude of the electron Fermi wavelength and the fullerene diameter, the description of the hybridization-induced scattering potential as a long-range potential is not adequate. In this case, the short-range approximation (sections 2 and 3) is more appropriate for a description of polaronic effects.

5. Conclusions

In conclusion, we have shown that the elastically soft subcomponent of peapods (fullerene molecules trapped inside a SWNT) can strongly influence low-temperature properties of resonant electron transport through short metallic peapods. If encapsulated C_{60}s do modify the
The electronic structure of metallic nanotubes (the effect was already observed for semiconducting peapods [5]), the mechanical degree of freedom associated with fullerene dynamics will influence, via polaronic effects, both the distribution of conductance peak amplitudes and peak spacings as a function of gate voltage. In our model, we considered independent vibrations of individual fullerenes (a disordered chain of $C_{60}$s inside a nanotube). This model predicts strong fluctuations and anomalous low-temperature behavior of Coulomb blockade conductance peaks. Such fluctuations have been experimentally observed [24].

One more question remains open, since our Hamiltonian, equation (4), does not include the effect of the scattering potentials due to the holes on the external shell on the nanotube electrons. In principle, the scattering of the electrons by these holes should be included. Our approximation, which neglects these effects, is based on two equally important observations.

The first observation is that there is experimental evidence [9] to suggest that electron transport through a peapod in a two-terminal conduction geometry, and in the presence of a gate electrode, is ballistic over the entire sample (whose length is around $\sim 400$ nm). In other words, the holes on the nanotube shell do not hinder ballistic electron transport.

The second observation is the following: the inclusion in the model of any topological defects (holes) in the tube shell would certainly affect the spectrum of the electrons in the nanotube and the level spacing. However, this would only result in a renormalization of the coupling constant $\lambda$, which in our model is a fitting parameter. The anomalous temperature dependence of conductance induced by vibrational dynamics of encapsulated fullerenes will not be affected.

Finally, we have also shown that the description of the hybridization-induced scattering potential as a long-range potential is not adequate to describe polaronic effects.

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