Photon-assisted transport in a carbon nanotube calculated using Green's function techniques

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We investigate the quantum transport through a single-walled carbon nanotube connected to leads in the presence of an external radiation field. We analyze the conductance spectrum as a function of the frequency and strength of the field. We found that above a critical value of the field intensity, an enhancement of the conductance, or suppressed resistance, as a function of the field strength occurs. The conductance increases displaying oscillations which amplitude shows a strong dependence on the field frequency. For low radiation energies in comparison with the lead–carbon-nanotube coupling energies, the oscillations evolve toward a structure of well defined steps in the conductance. We have shown that in this range of frequencies, the field intensity dependence of the conductance can give direct information of single-walled carbon nanotube energy spectra.

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I. INTRODUCTION

The electronic transport through carbon nanotubes (CNTs) has received much attention in the last decade due to the peculiar features of the band structure of these quasi-one-dimensional systems.[1,2] Depending on their diameter and chirality, CNTs can exhibit metallic or semiconducting behavior and therefore be promising candidates for new carbon-nanotube-based electronic devices. Some of them have already been realized, such as field-effect transistors,[3,4] field-emission displays,[5] and nanosensors.[6]

The quantum-mechanics behavior of the electronic transport in CNTs has been experimentally confirmed by Tans *et al.*[7] They showed that individual single-walled carbon nanotube (SWCNT) between two contacts behaves as coherent quantum wires, and Frank *et al.*,[8] have proven the quantization of the conductance of multiwalled carbon nanotubes. On the other hand, effects of time-dependent potentials on transport properties of CNTs have been previously studied by various authors.[9–11] Recently, Kim *et al.*[12] studied experimentally the microwave response of individual multiple CNT by finding an enhancement of the linear conductance under the microwave field.

In this work, we investigate the quantum transport through SWCNT connected to leads in the presence of an external radiation field. Specifically, we consider a time-dependent spatially uniform potential applied normal to the tube for modeling the effect of the radiation field. This problem is closely related to photon-assisted tunneling in nanostructures.[13] Basically, the external field induces the apparition of sidebands in the spectrum, and therefore the tunneling current is drastically modified.[14]

We solve the problem using standard nonequilibrium Green's function techniques. The conductance is calculated by the Landauer formula in terms of the transmission function, which is obtained from the retarded and advanced Green's functions of the SWCNT in the presence of the field, and the coupling of the nanotube to the leads.[15] We analyze the conductance spectra as a function of the frequency and amplitude of the external time-varying potential. We found that above a critical value of the radiation-field intensity, an enhancement of the conductance as a function of the field strength occurs. The conductance increases displaying oscillations with amplitudes strongly dependent on the field frequency. For low photon energies in comparison with the lead-CNT coupling energies, the oscillations evolve to a structure of well defined steps. This effect can be explained as due to the electric-field-induced sideband resonances that increase the local density of states at the Fermi energy, opening new channels for electronic transmission.

II. MODEL

The system (Fig. 1) under consideration is formed by a SWCNT embedded between two leads. The full system is modeled by the following Hamiltonian within a noninteracting picture, which can be written as

$$H = H_L + H_{CN} + H_{LCN}, \tag{1}$$

with

$$H_L = \sum_{q,\alpha} \varepsilon_{q_\alpha}(d^\dagger_{q_\alpha} d_{q_\alpha}),$$

$$H_{CN} = \sum_k \varepsilon_k (c^\dagger_k c_k),$$

$$H_{LCN} = \sum_{n=1,\alpha=l,r}^{N} (V_{q_\alpha,k} d^\dagger_{q\alpha} c_k + V^*_{q_\alpha,k} c^\dagger_k d_{q\alpha}), \tag{2}$$

where $c^\dagger_k$ is the creation operator of an electron at the state k of the carbon nanotube and $d^\dagger_{q,\alpha}$ is the corresponding operator of an electron in the state q of the right (α=R) or left (α=L) lead. Here, ε_k denotes the energy spectrum of a SWCNT.[2]

We will solve the problem using standard nonequilibrium Green's function techniques. In this formalism, the retarded and correlated Green's functions can be ex-

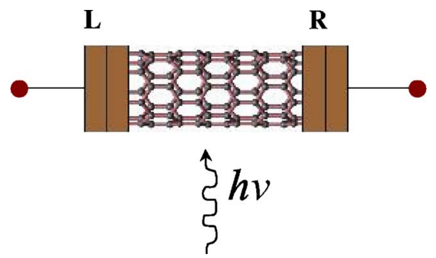

FIG. 1. (Color online) Schematized view of the CNT system considered.

pressed by $G_k^r(t,t') = -i\theta(t-t')\langle\{c_k(t), c_k^\dagger(t')\}\rangle$ and $G_k^<(t,t') = -i\langle c_k(t')c_k^\dagger(t)\rangle$. Here, the Green's functions G^r and $G^<$ are obtained from the Dyson equation $G^r = [(g^r)^{-1} - \Sigma^r]$ and Keldish equation $G^< = G^r\Sigma^< G^a$, where g^r is the unperturbed Green's function of the nanotube. The self-energies are given by $\Sigma^r = (-i/2)(\Gamma_L + \Gamma_R)$ and $\Sigma^< = (-i/2)(f_L\Gamma_L + f_R\Gamma_R)$, where $f_\alpha(\varepsilon)$ denotes the Fermi distribution. In the wide bandwidth approximation, the linewidth functions $\Gamma_\alpha(\varepsilon)$ are taken to be independent of the energy and energy levels. Once the Green's function G^r and $G^<$ are known, an expression for the current can be derived:[16]

$$I_\alpha = \frac{-2e}{\hbar}\int dt' \int \frac{d\varepsilon}{2\pi}\Im m \times\left(\sum_k \left\{ e^{-i\varepsilon(t'-t)/\hbar}\left\{\exp\left[(-i/\hbar)\int V(t'')dt''\right]\right\} \times\Gamma_\alpha(\varepsilon)[G^<(t,t') + f_\alpha(\varepsilon)G^r(t,t')]\right\}\right). \quad (3)$$

If the CNT is perturbed by a time-dependent, spatially uniform potential given by $V(t) = V_0\cos(\omega t)$,[14] the zero-voltage limit linear conductance will be given by[13]

$$G = \lim_{V\to 0}\frac{\langle I\rangle}{V} = \frac{2e^2}{\hbar}\int\frac{d\varepsilon}{2\pi}\sum_{nk} J_n^2\left(\frac{V_0}{\hbar\omega}\right) \times\left(-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right)\Gamma_L G_k^r(\varepsilon)\Gamma_R G_k^a(\varepsilon), \quad (4)$$

where $\langle I\rangle$ is the time-averaged current and $J_n(x)$ is nth-order Bessel function of the first kind. For this simple model, an effective density of states can be derived as follows,

$$\tilde{\rho}(\varepsilon) = \sum_n \left|J_n\left(\frac{V_0}{\hbar\omega}\right)\right|^2 \rho_0(\varepsilon - n\hbar\omega), \quad (5)$$

where $\rho_0(\varepsilon)$ is the bare density of states corresponding to the CNT in the absence of the perturbing potential. In the case of a $(n,0)$ CNT in the tight-binding approximation, this density of states can be expressed in analytic form as[17] shown in the Appendix. This equation can be physically interpreted as follows: photon absorption $(n>0)$ and emission $(n<0)$ can be viewed as creating an effective electron density of states at energies $\varepsilon_n = n\hbar\omega$ with a probability given by $|J_n(\frac{V_0}{\hbar\omega})|^2$.

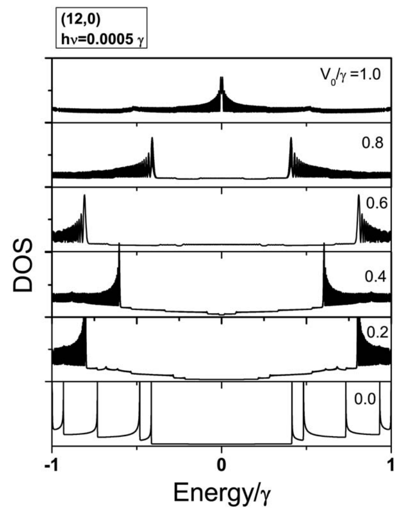

FIG. 2. Density of states for a (12,0) CNT under a radiation field of $h\nu = 0.0005\gamma$ and different values of the field strength.

III. RESULTS

In what follows, we will adopt the parameters $\gamma = 2.75$ eV, as the CNT hopping integral, and $\Gamma_L = \Gamma_R = \Gamma = 0.001\gamma$, as the lead-CNT coupling parameters. Figure 2 shows the density of states (DOS) of a zigzag CNT (12,0) as a function of the energy in units of γ for a particular photon energy $h\nu = 0.0005\gamma$ ($\nu = 332.5$ GHz) and for different values of V_0/γ, which essentially represents the radiation-field strength. It is clearly seen that the CNT pseudogap is strongly modified by the presence of the sideband resonances appearing due to the presence of the radiation field. These resonances are denser near the Fermi energy for increasing values of the field strength. This effect has strong influence on the system conductance due to the opening of new channels for electronic transmission, as we will see below.

The behavior of the DOS with the frequency of the radiation field is presented in Fig. 3 for the case of a semiconducting (5,0) CNT (upper panel) and for a metallic (6,0) CNT (lower panel). The radiation-field strength is taken as $V_0 = 0.3\gamma$, and different values of the photon energy are considered. We note that for the semiconducting tube, the changes of the DOS near the Fermi energy are more noticeable than that for the metallic tube; in fact, the gap of (5,0) becomes closed for frequencies of the order of Γ.

In Fig. 4, we have displayed the normalized linear conductance G/G_0, where $G_0 = 2e^2/h$ is the quantum of conductance, for a semiconducting (11,0) and a metallic (12,0) CNT as a function of the intensity of the radiation field. We have plotted the corresponding conductance for different photon energies $h\nu = 0.0005\gamma$ (solid line), $h\nu = 0.005\gamma$ (magenta online), and $h\nu = 0.05\gamma$ (dashed blue line). For semiconducting tubes, the gap in the conductance becomes closed as a consequence of the sideband resonances in the DOS induced by the presence of the radiation field. In both kinds of tubes, the

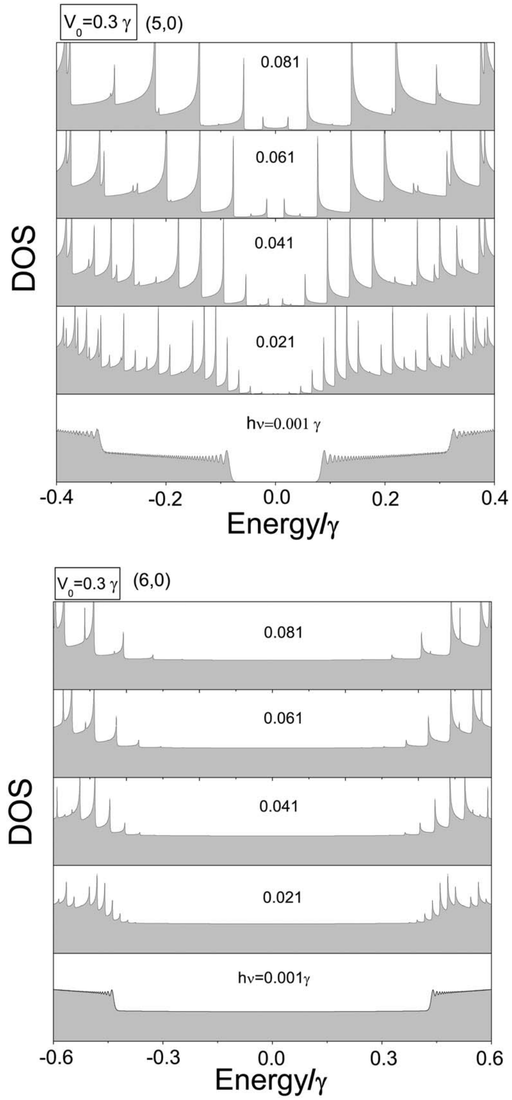

FIG. 3. Density of states for (5,0) (upper panel) and (6,0) (lower panel) CNTs under a radiation-field strength of $V_0=0.3\gamma$ and different values of the field frequency.

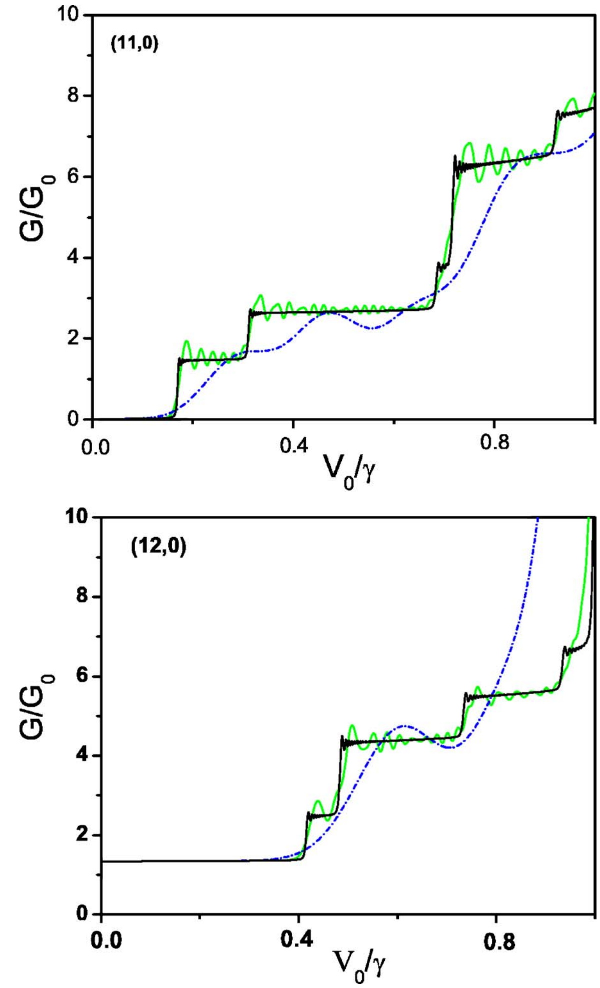

FIG. 4. (Color online) Normalized linear conductance of a (11,0) (upper panel) and a (12,0) (lower panel) CNT as a function of the oscillating field strength in unit of γ; solid black line corresponds to $h\nu=0.0005\gamma$, solid green (gray) line to $h\nu=0.005\gamma$, and blue (gray) dashed line to $h\nu=0.05\gamma$.

strong enhancement of the conductance as function of the intensity of the radiation field can be observed. For low frequencies, $\nu<\Gamma/h$, the conductance presents a very well-defined structure of steps. For increasing frequencies, some oscillations appear inducing a complete suppression of the step features for frequencies $\nu\gg\Gamma/h$.

To analyze in more detail the dependence of the conductance with the field frequency, we have plotted in Fig. 5 the conductance as a function of the photon energy for three different values of the field strength for a (12,0) and a (11,0) CNT. It can be observed that the conductance as a function of the radiation frequency presents two regimens: one for low frequencies ($\nu<\Gamma/h$), in which the conductance is almost independent of the frequency for both kinds of nanotubes, and the other for higher frequencies, for which the conductance presents an oscillatory response with the frequency. In the case of the metallic (12,0) CNT, the conductance is almost independent of the field frequency for the particular value of the radiation strength chosen ($V_0=0.3\gamma$). This was also evidenced in Fig. 4, where due to this value, of V_0 is lower than the pseudogap of the CNT. In the case of the semiconducting tube, the value of $V_0=0.3\gamma$ is greater than the (11,0) gap, and the conductance with the frequency oscillates with a very little amplitude. For increasing field strengths, the conductance oscillates with the frequency around a fixed value.

The step structure in the conductance for low frequencies can be understood because in that range of frequencies, the system is found in a quasistatic regime, and the spectrum as a function of the strength of the radiation field V_0 is just linearly shifted. As the field intensity increases, the Van Hove singularities cross the Fermi energy, leading to an abrupt increase in the conductance. In fact, each step in the conductance reflects the energy position of the corresponding Van Hove singularity of the nanotube DOS. Figure 6 shows the normalized conductance versus the strength of the radiation field for a (15,0) CNT. There we have included the corresponding DOS in the same energy range.

In Fig. 7, we show the behavior of the normalized resistance versus radiation-field strength with the nanotube ra-

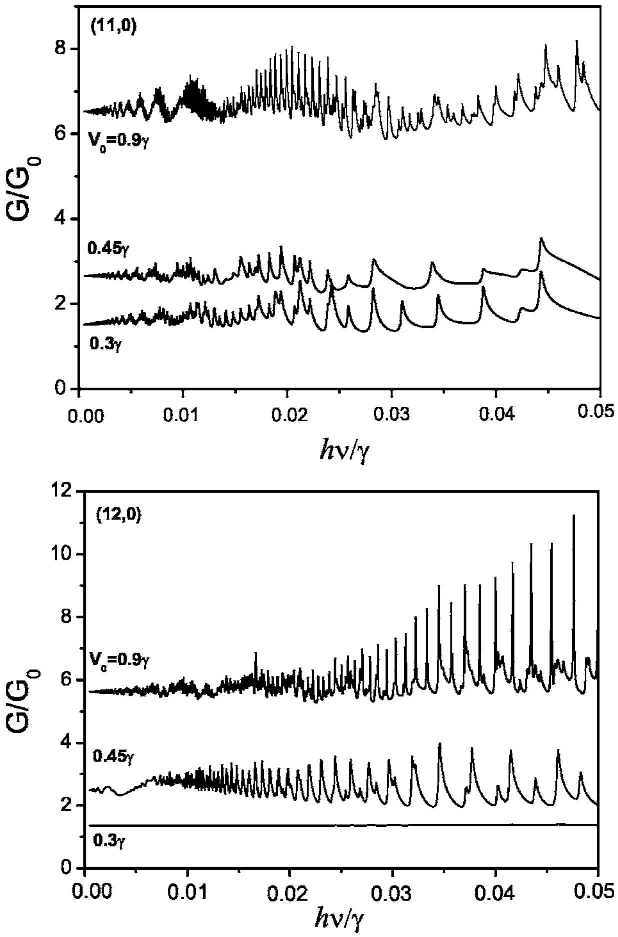

FIG. 5. Normalized conductance of (12,0) (upper panel) and (11,0) (lower panel) CNTs as a function of the energy photon, in units of γ, for $V_0=0.3\gamma$, $V_0=0.45\gamma$, and $V_0=0.9\gamma$.

dius. The figure displays plots for (a) (9,0) and (b) (18,0) metallic nanotubes. In both cases, the step structure is clearly manifested with increasing number of steps for larger radii. This step structure is a reflex of the quasi-one dimensional density of states of the CNT. These results can be compared

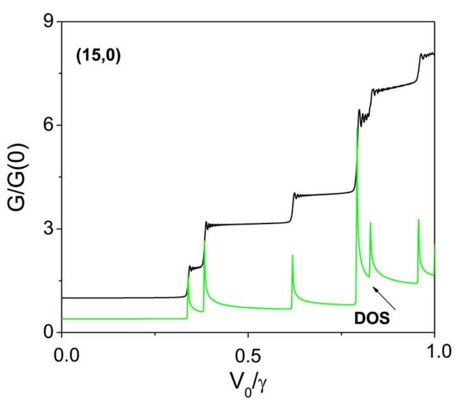

FIG. 6. (Color online) Normalized conductance of a (15,0) CNT as a function of the oscillating field strength, in units of γ, for $h\nu=0.0005\gamma$. The corresponding DOS of the CNT is also plotted in the same energy range.

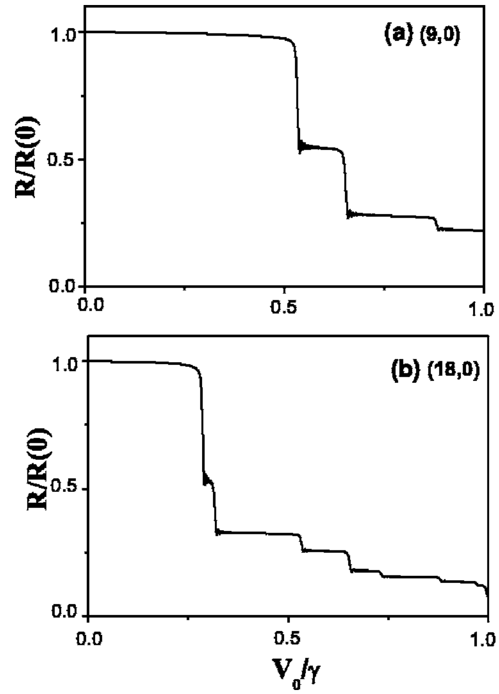

FIG. 7. Normalized resistance for CNTs of different diameters as function of the oscillating field strength, (a) (9,0) CNT and (b) (18,0) CNT, for $h\nu=0.0005\gamma$.

with the experimental results of Kim *et al.*,[12] who studied the microwave response of an individual CNT. They effectively found that the resistance decreases as a function of the radiation-field power regardless of the frequency. In their experiment, the step structure is not observed because they studied a multiple nanotube of about 25 nm wide. In this case, the quasi-one-dimensional character of the CNT DOS is completely suppressed.

IV. SUMMARY

We have investigated quantum transport through CNTs connected to leads in the presence of an external radiation field. We studied the conductance spectra as a function of the frequency and of the field strength. We found that above a critical value of the field strength, an enhancement of the conductance, or suppressed resistance, as a function of the field intensity occurs. The conductance increases displaying oscillations which amplitude shows a strong dependence on the frequency of the oscillating field. For low radiation energies in comparison with the lead-CNT coupling energies, the oscillations evolve toward a structure of well defined steps in the conductance. We have shown that in this range of frequencies, the field intensity dependence of the conductance can give direct information of CNT energy spectra.

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APPENDIX

The Green's function of a graphite sheet is given by[17]

$$G^r(\varepsilon,\mathbf{k}) = \frac{\varepsilon/\gamma}{\varepsilon^2 - 3 - 2\cos(2k_x a) - 4\cos(k_x a)\cos(3k_y b)}. \tag{A1}$$

To describe a zigzag CNT, it is enough to impose periodic boundary conditions along the direction of the chiral vector. Then, $k_x a = \frac{\pi}{n} j$, with $j = 0 - 2n$ and $-\pi/3b < k_y < \pi/3b$. To obtain the Green's function in the real space, we apply the Fourier transform to $G^r(\varepsilon,\mathbf{k})$,

$$G^r(\varepsilon,l,m) = \frac{(6ab)\varepsilon}{4\pi^2}\sum_{j=0}^{2n}\int_{-\pi/3b}^{\pi/3b} dk_y \frac{e^{-i(\pi/n)jl}e^{-3ik_x mb}}{\varepsilon^2 - 3 - 2\cos\left(2\frac{\pi}{n}j\right) - 4\cos\left(\frac{\pi}{n}j\right)\cos(3k_y b)}. \tag{A2}$$

The integral over k_y can be solved to obtain an analytical expression for the Green's function,

$$\rho_0(\varepsilon) = \frac{1}{\pi}\Im m \sum_{j=0}^{2n}\left(\frac{(-2/3)(\varepsilon + i0^+)}{i\pi\sqrt{16\cos^2\left(\frac{\pi}{n}j\right) - \left[(\varepsilon + i0^+)^2 - 1 - 2\cos^2\left(\frac{\pi}{n}j\right)\right]^2}}\right). \tag{A3}$$

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