AC Conductivity of Metallic Carbon Nanotubes (CNTs) Exposed to a DC Field

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Abstract

The AC conductivity of a carbon nanotube (CNT) is derived and it is shown that it can become negative when the CNT is exposed to a DC axial field in addition to the AC field. For this purpose, the Boltzmann transport equation (BTE) is solved within the relaxation time approximation (RTA) by separating the AC and DC contributions. The near-equilibrium approximation is used for the DC part of the carrier distribution. The AC carrier distribution and the AC conductivity are subsequently found via a semi-analytical procedure. Absolute negative AC conductivity is found at for a DC field above 10^5 V/m, which is a promising result toward enabling CNT traveling-wave amplifiers.

1 Introduction

Ever since their discovery, carbon nanotubes (CNTs) have shown remarkable electronic properties [1, 2], such as high electron mobility [3] and ambipolarity [4], that made them a subject of investigation by many researchers. These properties have already been exploited in several CNT devices, high-speed field-effect transistors possibly being the most important of them [5]. Furthermore, theoretical and experimental works have shown the existence of non-linear phenomena in CNTs, such as negative differential DC conductivity [6], making CNTs suitable for high-frequency generating nano-devices.

In [7], Maksimenko *et al.* treated the combined DC-AC CNT problem, and found instabilities in the AC field for a CNT exposed to a high axial DC field, and they speculated that this effect could lead to amplification of the AC field. However, the analysis conducted in [7] was based on the crude assumption of a helical CNT lattice, barely approximating the actual hexagonal structure of the CNT.

In this contribution, using the CNT tight-binding band-structure model [1], we derive the AC conductivity of CNTs exposed to an axial DC field. For this purpose, we solve the Boltzmann transport equation (BTE) under the commonly used relaxation time approximation (RTA) [8], and compute the AC conductivity as a function of the applied DC field. The analysis relies on the separation of the DC and AC distributions, leading to specific expressions for the AC distribution and conductivity. The near-equilibrium approximation is used, providing quantitative and qualitative descriptions of the problem for DC fields below and beyond 10^5 V/m, respectively. Absolute negative AC conductivity is found for DC fields above 10^5 V/m, which suggests amplification of the AC signal at the expense of the DC energy.

2 Boltzmann Transport Equation and Carrier Distribution

Let us consider a metallic zigzag CNT of chiral vector $(n = 3q, 0)$, where n and q are integers [1]. Neglecting chiral corrections, a reasonable approximation for the electronic dispersion relation of the doubly-degenerated band passing through the Fermi level is given by the linear function

$$\varepsilon(p_z) \approx \frac{3b\gamma_0}{2\hbar}|p_z| = v_f|p_z|, \tag{1}$$

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where ε is the energy, p_z is the z component of the crystal momentum which corresponds to the axis of the CNT, $b = 1.42$ Å is the carbon interatomic distance, γ_0 is the overlap integral, evaluated empirically to be around 2.7 eV, and $v_f = 8.73 \times 10^5$ m/s is the Fermi velocity [9].

In order to find the AC conductivity in the presence of a DC bias, we need the AC carrier distribution through the BTE. Under the RTA, the 1D BTE is written as

$$\frac{\partial f}{\partial t} + v_z \frac{\partial f}{\partial z} + F_e \frac{\partial f}{\partial p_z} = -\frac{f - f_0}{\tau}, \tag{2}$$

where $f(p_z, z, t)$ is the carrier distribution, f_0 is the equilibrium carrier distribution, $v_z(p_z) = \partial\varepsilon/\partial p_z$ is the electron wave packet group velocity and $\tau = 3 \times 10^{-12}$ s is the scattering time in CNTs. The force exerted by the DC and AC fields on the electrons is

$$F_e = -e(E_z^{dc} + E_z^{ac}), \tag{3}$$

where E_z^{dc} is the DC electric field applied along the axis and assumed constant along the CNT, and E_z^{ac} is the AC electric field. In general, $E_z^{ac} = \mathrm{Re}[E_{z0}^{ac} e^{j(hz - \omega t)}]$, where E_{z0}^{ac} is the AC electric field magnitude, h the propagation constant along the CNT and ω the angular frequency. Assuming negligible non-local effects, h is set to zero. The equilibrium distribution f_0 is the Fermi-Dirac distribution $f_0 = 1/[1 + e^{\varepsilon/(k_B T)}]$, which upon substitution of ε from (1) becomes

$$f_0(p_z) = \frac{1}{1 + e^{v_f |p_z|/(k_B T)}}. \tag{4}$$

We next separate the distribution into its DC and AC parts by writing $f = f^{dc} + f^{ac} = f^{dc} + \mathrm{Re}[f_0^{ac} e^{-j\omega t}]$ [10]. Assuming steady-state and spatial uniformity for the DC distribution we have $\partial f^{dc}/\partial t = 0$ and $\partial f^{dc}/\partial z = 0$, respectively. Inserting (3) into (2), using the aforementioned assumptions, and separating the DC and AC parts, we find the equations

$$\frac{\partial f^{dc}}{\partial p_z} - \frac{1}{\Delta p_z} f^{dc} = f_0, \tag{5a}$$

$$\frac{\partial f_0^{ac}}{\partial p_z} - \frac{\Omega}{\Delta p_z} f_0^{ac} = -R_a \frac{\partial f^{dc}}{\partial p_z}, \tag{5b}$$

where $\Delta p_z = e\tau E_z^{dc}$, $\Omega = 1 - j\tau\omega$ and $R_a = E_{z0}^{ac}/E_z^{dc}$. Equation (5a) is known as the 1-D drift equation. It can be solved using the near equilibrium approximation by shifting the equilibrium distribution function f_0 in the momentum space by exactly the amount of momentum Δp_z given to each electron [8]. Thus, from (4),

$$f^{dc}(p_z) \approx f_0(p_z + \Delta p_z) = \frac{1}{1 + e^{v_f |p_z + \Delta p_z|/(k_B T)}}. \tag{6}$$

The AC distribution, found as the solution to the linear ordinary first-order differential equation (5b), is given by [11]

$$f_0^{ac}(p_z) = e^{\Omega p_z/\Delta p_z} \left[\int_0^{p_z} -R_a \frac{\partial f^{dc}(p_z')}{\partial p_z'} e^{-\Omega p_z'/\Delta p_z} dp_z' + f_0^{ac}(0) \right]. \tag{7}$$

Applying integration by parts we get

$$f_0^{ac}(p_z) = -R_a e^{\Omega p_z/\Delta p_z} \left[f^{dc}(p_z) e^{-\Omega p_z/\Delta p_z} \Big|_0^{p_z} + \frac{\Omega}{\Delta p_z} \int_0^{p_z} f^{dc}(p_z') e^{-\Omega p_z'/\Delta p_z} dp_z' \right] + f_0^{ac}(0) e^{\Omega p_z/\Delta p_z}. \tag{8}$$

To find $f_0^{ac}(0)$ we first apply the boundary condition $\lim_{p_z \to \infty} f_0^{ac}(p_z) = 0$, which ensures the absence of carriers with infinite momentum. Second, noting that $\mathrm{Re}\{\Omega\} > 0$, we find that $\lim_{p_z \to +\infty} e^{-\Omega p_z/\Delta p_z} f_0^{ac}(p_z) = 0$. Applying this condition to (8) yields the sought after result

$$f_0^{ac}(0) = R_a \left[-f^{dc}(0) + \frac{\Omega}{\Delta p_z} \int_0^{\infty} f^{dc}(p_z) e^{-\Omega p_z/\Delta p_z} dp_z \right]. \tag{9}$$

Substituting (9) in (8) yields the AC distribution,

$$f_0^{ac}(p_z) = -R_a f^{dc}(p_z) + R_a \frac{\Omega}{\Delta p_z} \int_{p_z}^{\infty} f^{dc}(p'_z) e^{-\Omega p'_z/\Delta p_z} dp'_z. \tag{10}$$

The integral in (10) is computed numerically to find f_0^{ac}.

3 AC Conductivity

The general relation for the surface current density is $J_z = -2e/(2\pi\hbar)^2 \iint_{BZ} f(p_z) v_z(p_z) dp_z dp_\phi$ where p_ϕ is the azimuthal component of the momentum. However, p_ϕ is quantized in a CNT due to transversal confinement. Moreover, for a zigzag CNT, $p_\phi = (2\pi\hbar s)/(\sqrt{3}nb)$ where s is the azimuthal number [1]. We can thus write

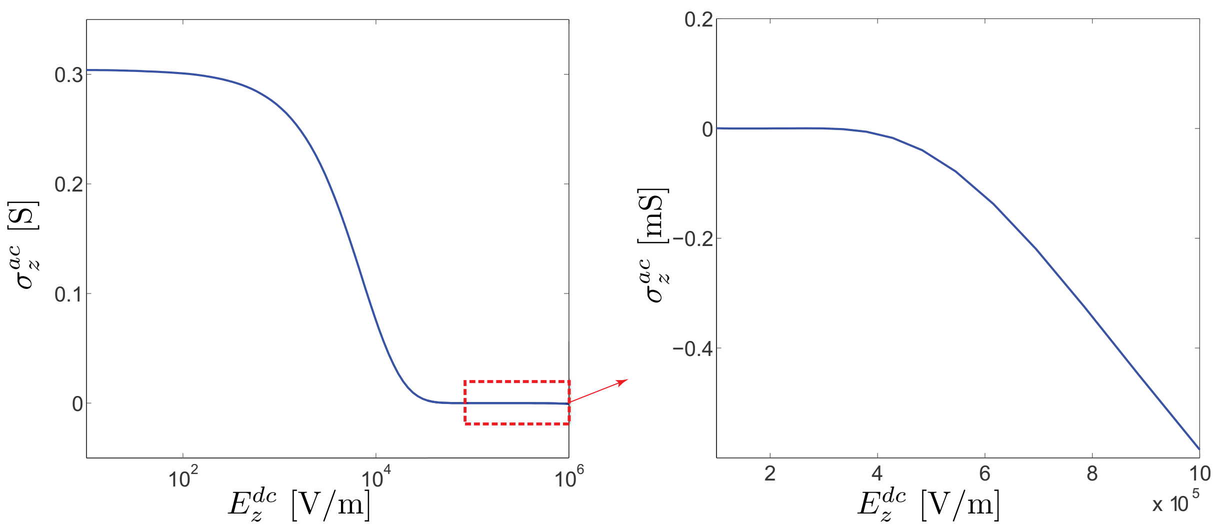
$$J_z^{ac} = \frac{-2e}{(2\pi\hbar)^2} \frac{2\pi\hbar}{\sqrt{3}nb} \sum_{s=1}^{2n} \int_{-u}^{u} f^{ac}(p_z, s) v_z(p_z, s) dp_z, \tag{11}$$

where $u = \pi\hbar/3b$ is the Brillouin zone boundary. In a metallic zigzag CNT, only the sub-bands considered in (1), namely $s = 2n/3$ and $s = 4n/3$, contribute to conduction. Thus, the final expression for the AC current density becomes

$$J_{z0}^{ac} = \frac{-2e}{\sqrt{3}nb\pi\hbar} \left[\int_{-u}^{0} -v_f f_0^{ac}(p_z) dp_z + \int_{0}^{u} v_f f_0^{ac}(p_z) dp_z \right], \tag{12}$$

where J_{z0}^{ac} is the current magnitude.

Fig. 1 plots the AC conductivity $\sigma_z^{ac} = J_{z0}^{ac}/E_{z0}^{ac}$ versus E_z^{dc} for a (6,0) CNT at 1 GHz. It is clearly seen in Fig. 1(b) that σ_z^{ac} takes negative values when $E_z^{dc} > 2 \times 10^5$ V/m, indicating the possibility of AC amplification in a metallic CNT at high DC fields.



(a) (b)

Figure 1: AC conductivity for a (6,0) CNT with respect to applied DC bias field. (a) Wide view showing the transition from the low DC field positive conductivity region to the large DC field negative conductivity region. (b) Zoomed view on the negative conductivity region.

4 Conclusion

It has been shown through a semi-classical BTE analysis that a metallic zigzag CNT takes a negative AC conductivity when biased with sufficiently high DC fields, rendering it a possible candidate for a novel type of traveling-wave amplifiers. This work presents a motivation to explicitly study the amplification, which will be the goal of future work.

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