# Enhanced nonlinear conductivity due to hot-electron injection in carbon nanotubes

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## ABSTRACT

We have theoretically obtained an expression for the current density in a terahertz field due to hot-electron injection in carbon nanotubes. The injection modifies the stationary distribution function and leads to a qualitative change in the behavior of the current-voltage characteristics and causes absolute negative conductivity. We compared the current-voltage characteristic behavior at different injection rates and observed a drastic change in the current density and absolute negative conductivity values. We propose that carbon nanotubes with hot-electron injection may be useful for high-frequency applications. 2023 10:0

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## **1. INTRODUCTION**

Recently, increasing attention has been focused on the behavior of hot-electron injection in carbon nanotubes (CNs).<sup>1-3</sup> This is essentially due to its importance in understanding various nonlinear kinetic effects and the band structure.<sup>1-3</sup> Interesting dynamical behaviors that can be observed in biased CNs with hot-electron injection include Bloch oscillations, high frequency conductivity, negative differential conductivity, absolute negative conductance, etc. The processes to obtain hot electron are by electrical injection, optical excitation, and high energetic particles.<sup>4–11</sup> These techniques have created opportunities and made it feasible to generate hot electrons to explore their influence on thermoelectric, galvanomagnetic, piezoelectric, and thermomagnetic properties of other materials.<sup>4–11</sup> The objectives of the study have been given. First, to solve the Boltzmann equation in the presence of a static electric field with hot-electron injection and to determine the distribution function in the time varying fields. Second, to obtain the expressions for the THz-field rectification due to hot-electron injection in CNs. Finally, to show that the injection modifies the distribution function and leads to enhance nonlinearity.

# 2. THEORY

The motion of the quasiparticles in the presence of external field in CNs with hot-electron injection can be described by the

09:15 semiclassical Boltzmann transport equation with constant relaxation time which is satisfied by the time-dependent distribution function that defines the macroscopic average states of electron in Ref. 12 as

$$\frac{\partial f}{\partial t} + eE\frac{\partial f}{\partial p} = -\frac{f-F}{\tau} + Q\delta(p-p') - \frac{Q}{n_0}(f-F)$$
(1)

with

$$F(\varphi_{\mu}) = \frac{n_0}{2\pi\hbar I_0(x_{\gamma})I_0(x_{\xi})} \prod_{\mu} d_{\mu} \sum_{l=-\infty}^{\infty} I_l(x) e^{il\varphi_{\mu}}$$

Here,  $x_{\mu} = \Delta_{\mu}/(kT)$ ,  $\varphi_{\mu} = p_{\mu}d_{\mu}/\hbar$ ,  $\omega_{E,\mu} = eE_{\mu}d_{\mu}/\hbar$ . The index  $\mu(=\xi;\gamma)$ denotes the tubular axis and the base helix, respectively. f is the distribution function, F is the equilibrium distribution function, p is the electron dynamical momentum,  $\tau$  is the electron relaxation time approximation and further assumed constant, e is the electron charge,  $Q/n_0$  is the hot-electron pumping frequency with Q as the rate of injection of hot electron, and p' is the injection momentum. The spectrum of the electrons in the miniband of the chiral CNs in

a standard tight-binding approximation<sup>13–16</sup> is

$$\varepsilon(p) = \varepsilon_0 - \Delta_{\xi} \cos\left(\frac{p_{\xi} d_{\xi}}{\hbar}\right) - \Delta_{\gamma} \cos\left(\frac{p_{\gamma} d_{\gamma}}{\hbar}\right), \tag{2}$$

where  $\varepsilon_0$  is the energy of an outer-shell electron in an isolated carbon atom,  $\Delta_{\xi}$  and  $\Delta_{\gamma}$  are the real overlapping integrals for jumps along the respective coordinates,  $p_{\xi}$  and  $p_{\gamma}$  are the components of momentum tangential to the base helix and along the nanotube axis, respectively,  $\hbar$  is the Planck's constant while  $d_{\xi}$  and  $d_{\gamma}$  are the distances along the axis and helix, respectively.

Expanding  $\varepsilon(p)$  in Fourier series due to its periodicity in the quasimomentum, we have

$$\varepsilon(p) = \sum_{\kappa=-1}^{1} \varepsilon(\kappa, p) e^{i\kappa\varphi_{\mu}}, \qquad (3)$$

where  $\varepsilon(\kappa, p)$  is the coefficient of Fourier series.  $\kappa$  is the infinite integer.

The electron quasiclassical velocity component  $v(p_{\mu})$  is obtained in Refs. 1–4,

$$\nu(p_{\mu}) = \frac{\partial \varepsilon(p)}{\partial p_{\mu}} = \sum_{\kappa=-1}^{1} i \kappa \varepsilon(\kappa, p) e^{i \kappa \varphi_{\mu}}.$$
 (4)

The electron fluxes along the tubular axis and the base helix are given as  $^{\rm l3-16}$ 

$$\prod_{\xi} = \frac{2e}{(2\pi\hbar)^2} \iint v_{xi}(p_{xi})f(p,t)dp_{xi}dp_{\gamma},$$
(5)

$$\prod_{\gamma} = \frac{2e}{(2\pi\hbar)^2} \iint v_{\gamma}(p_{\gamma}) f(p,t) dp_{xi} dp_{\gamma}, \tag{6}$$

where the integration is done over the first Brilloiun zone. The expressions for the axial and the circumferential components are as in Refs. 13-16:

$$j_{\xi} = \prod_{\xi} + \prod_{\gamma} \sin \theta_h, \tag{7}$$

$$j_{\gamma} = \prod_{\gamma} \cos \theta_h. \tag{8}$$

Solving Eq. (1) with  $E = E_0 + E_1 \cos \omega t$  and substituting the solution together with Eqs. (4) and (5) into Eqs. (6) and (7), we obtained for Eqs. (7) and (8) the following current expressions:

$$j_{\xi} = j_{\xi,0} \sum_{l=-\infty}^{\infty} \frac{j_l^2 [\beta_{\xi}(\omega_{E,\xi}\tau + l\omega\tau)]}{1 + 2\eta\tau + (\eta\tau)^2 + (\omega_{E,\xi}\tau + l\omega\tau)^2} + j_{\gamma,0} \sum_{l=-\infty}^{\infty} \frac{j_l^2 [\beta_{\gamma}(\omega_{E,\gamma}\tau + l\omega\tau)]}{1 + 2\eta\tau + (\eta\tau)^2 + (\omega_{E,\gamma}\tau + l\omega\tau)^2} \times \left[ 1 + \eta\tau \left( \frac{I_0(x_{\gamma})}{I_1(x_{\gamma})} e^{-il\varphi_{\gamma}} + 1 \right) \right] \sin^2 \theta_h,$$
(9)

$$j_{\gamma} = j_{\gamma,0} \sum_{l=-\infty}^{\infty} \frac{j_{l}^{2} [\beta_{\gamma}(\omega_{E,\gamma}\tau + l\omega\tau)]}{1 + 2\eta\tau + (\eta\tau)^{2} + (\omega_{E,\gamma}\tau + l\omega\tau)^{2}} \times \left[1 + \eta\tau \left(\frac{I_{0}(x_{\gamma})}{I_{1}(x_{\gamma})}e^{-il\varphi_{\gamma}} + 1\right)\right] \sin \theta_{h} \cos \theta h.$$
(10)



**FIG. 1.** Plots of normalized dc current density  $j_{\mu} J_{\mu,0}$  as a function of a dimensionless amplitude  $\beta_{\mu}$  when  $\eta \tau = 0.05$ ,  $\varphi = 0.9\pi$  and  $\eta = 0.2$ , 0.5, 5.0; for (a) axial axis and (b) circumferential axis.



**FIG. 2.** Plots of normalized dc current density  $j_{\mu}/j_{\mu,0}$  as a function of a dimensionless amplitude  $\beta_{\mu}$  when  $\omega \tau = 0.5$ ,  $\varphi = 0.9\pi$  and  $\eta \tau = 0.01$ , 0.03, 0.05; for (a) axial axis and (b) circumferential axis.

Here  $x_{\mu} = \Delta_{\mu}/(kT)$ ,  $\eta = Q/n_0$ ,  $\beta_{\mu} = eE_{1,\mu}d_{\mu}/(\hbar\omega)$  and

$$\dot{h}_{\mu,0}=rac{n_0e\Delta_\mu d_\mu}{\hbar}rac{I_1(x_\mu)}{I_0(x_\mu)}.$$

The Coulomb electron-electron interaction has been neglected in our approach. It has been established that the short-range Coulomb electron-electron interaction, typical for quasi-onedimensional CNTs, have only weak effects especially at high temperatures.<sup>17,18</sup> The effect of space charge inside CNs was neglected, since space charge injection and accumulation in CNs are suppressed to a large extent when strength of the external electric field is less than 40V/ $\mu$ m.<sup>19,20</sup>

## **3. RESULTS AND DISCUSSIONS**

We theoretically investigate enhanced nonlinear conductivity due to hot-electron injection in chiral carbon nanotubes. The effect is in essence may be attributed to the nonparabolicity of the energy bands and the inherent chiral electronic properties of the carbon nanotubes. The nonlinearity is analyzed based on the normalized current density  $j_{\mu}/j_{\mu,0}$  as a function of the strength of the ac amplitude  $\beta_{\mu}$ . Current density as a function of the ac amplitude  $\beta_{\mu}$  at different injection rate with  $\Delta_{\xi} = 0.024$  eV,  $d_{\xi} = 2$  nm,  $\tau = 3.0$  ps,  $E_{\xi} = 5.6$ V/µm and with  $\Delta_{\gamma} = 0.018$  eV,  $d_{\xi} = 2$  nm,  $\tau = 3.0$  ps,  $E_{\xi} = 10.97$ V/µm at room temperature when  $\theta = 4^{\circ}$  are shown in Figs. 1 and 2, respectively.

Current-voltage characteristics obtained from Eqs. (9) and (10) are presented in Fig. 1 for (a) axial component and (b) circumferential component. From the figures, the normalized current density  $j_{\mu}/j_{\mu,0}$  is plotted as a function of the strength of the ac amplitude  $\beta_{\mu}$  for different values of  $\omega \tau$  when dimensionless injection rates  $\eta \tau = 0.05$ . It can be clearly observed that the behavior is similar in

the axial and circumferential components for each  $\omega \tau$  value. In the region of strong scattering  $\omega \tau < 1$ , the normalized current density  $j_{\mu}/j_{\mu,0}$  is positive but decreases with increasing the strength of the ac amplitude  $\beta_{\mu}$ . However, for the case of weak scattering, normalized current density decreases strongly with increasing ac amplitude and then oscillates around the current density  $j_{\mu}/j_{\mu,0}$  with intervals of absolute negative conductivity.

Figure 2 illustrates the normalized current density  $j_{\mu}/j_{\mu,0\overline{c}}$  dependence on the strength of the ac amplitude  $\beta_{\mu}$  for difference injection rates  $\eta$  when  $\omega \tau = 5.0$ . It has been shown that the behavior is similar in the axial and circumferential components. We observe that as injection rates  $\eta$  increases, the normalized current density  $j_{\mu}/j_{\mu,0}$  values increase and the region of the occurrence of the absolute negative conductivity slightly shifts to the low value of the ac amplitude  $\beta_{\mu}$  and the magnitude of the value of the absolute negative conductivity is also increased (see Fig. 2). We observed that with high injection rate, enhanced nonlinear conductivity is observed in a CNs even at a room temperature. We note that the current density values and the absolute negative conductivity for the axial carbon nanotubes significantly exceed the corresponding values and regions of the circumferential nanotubes.

## 4. CONCLUSION

In summary, strong nonlinear effects in CNs with hot-electron injection are investigated theoretically. The dependence of the current density  $j_{\mu}/j_{\mu,0}$  on the strength of the ac amplitude  $\beta_{\mu}$  is considered and the influence of  $\eta$  is taken into account. We compared the current-voltage characteristic behavior at different injection rates and noted a drastic change in the values of the current density and the absolute negative conductivity. We propose that carbon nanotubes with hot-electron injection may be useful for strong nonlinear effects.

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