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Rectification due to harmonic mixing of two coherent electromagnetic waves with commensurate frequencies in carbon nanotubes

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Abstract. We report on a theoretical investigation of carbon nanotubes subjected to a pure alternating electric field consisting of two phase-shifted harmonic fields of frequencies $\omega_1 = \Omega$ and $\omega_2 = 2\Omega$ (harmonic mixing) without any direct current bias. We employed a tight-binding approximation for the description of the energy bands of the carbon nanotubes and the Boltzmann transport equation with constant relaxation time approximation. The results are compared to that of a superlattice under similar conditions. The results indicate a direct current generation by the carbon nanotubes due to the harmonic mixing. The described effect is in essence, due to the nonlinearity associated with the non-parabolicity of the electron energy band, which is greater in the carbon nanotubes than the superlattices. The strong effect observed in the carbon nanotubes is attributed to the stark components and the specific dispersion law inherent in hexagonal crystalline structure of the carbon nanotubes.

1 Introduction

Carbon nanotube (CNT) is a cylindrical molecular structure with nanometer diameter and micrometer length [1]. Since the discovery by Iijima in 1991 [2], the interest in these quasi-one-dimensional monomolecular structures has grown exponentially, mainly due to their unique thermal, chemical and physical properties [3]. These properties depend on the fundamental indices (n,m) of the CNTs. The indices (n,m) determine the diameter and the chiral angle of the CNT. As n and m vary, the conduction ranges from metallic to semiconducting [4], with an inverse diameter dependent band gap of $\leqslant$1 eV [5].

The study of CNTs is now an active research area, which could lead to the development of technologically advanced devices [6]. CNTs show strong nonlinear response to high frequency (HF) fields governed by a strong nonparabolic dispersion law [6]. Therefore CNTs can be used for generation of harmonics of electromagnetic radiation [7–10]. However, to the best of our knowledge, rectification of sinusoidal wave with two coherent waves with commensurate frequencies has not been investigated in CNTs.

In fact several mechanisms of nonlinearity could be responsible for the wave mixing in semiconductors [11–14]. Important among them is the heating mechanism where the nonlinearity is related to the dependence of the relaxation constant on the electric field [13–17]. Goychuk and Hänggi [18] have suggested another scheme of quantum rectification using wave mixing of an alternating electric field and its second harmonic in a single miniband superlattice (SL). Their approach is based on the theory of quantum ratchets. The necessary conditions needed to observe a dc behavior in such a system included a dissipative (quantum noise) and an extended periodic system [18].

In this paper we focus on the mechanism of nonlinearity due to the nonparabolocity of the electron energy spectrum in SLs and CNTs. In superlattices, the theory of wave mixing based on the solution of the Boltzmann equation has been studied [19–24]. However, none of these reports considered the case of a time dependent electric field, $E(t) = E_1 \cos \omega_1 t + E_2 \cos(\omega_2 t + \theta)$. Mensah et al. were the first to report on the use of such alternating current in SLs [25].

In this work, we investigate for the first time the possibility of the generation of a direct current (dc) in CNTs due to a wave mixing of two coherent electromagnetic radiations of commensurate frequencies. We compared the dc generation in a zigzag CNT, an armchair CNT and a SL, subjected to an ac field with its second harmonic. We observed stronger effects in the CNTs than in the SL, due

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to the strong non-parabolicity of the electron energy band in the CNTs.

This work is organized as follows: Section 1 is the introduction, we establish the theory and solution of the problem in Section 2 and discuss the results and draw conclusions in Section 3.

2 Theory

We consider an undoped single-wall CNT subjected to two harmonic fields (harmonic mixing),

$$E(t) = E_1 \cos \omega_1 t + E_2 \cos(\omega_2 t + \theta). \quad (1)$$

We use the semiclassical approximation in which π-electrons are considered as classical particles with the dispersion law extracted from quantum theory. Considering the hexagonal crystalline structure of zigzag CNTs with tight binding approximation, the dispersion relation is given as [3]:

$$\begin{aligned}\varepsilon\left(s\Delta p_\varphi, p_z\right) &\equiv \varepsilon_s(p_z)\\ &= \pm\gamma_0 \left[1 + 4\cos(ap_z)\cos\left(\frac{a}{\sqrt{3}}s\Delta p_\varphi\right)\right.\\ &\quad \left. +4\cos^2\left(\frac{a}{\sqrt{3}}s\Delta p_\varphi\right)\right]^{1/2}. \quad (2)\end{aligned}$$

Here $\gamma_0 \sim 3.0$ eV is the overlapping integral, p_z is the axial component of quasimomentum, Δp_φ is the transverse quasimomentum level spacing and s is an integer. The expression for a in equation (2) is given as $a = 3b/2\hbar$ with the C-C bond length $b = 0.142$ nm and $\hbar = h/2\pi$ is the Plank's constant. The − and + signs correspond to the valence and conduction bands, respectively. Due to the transverse quantization of the quasi-momentum, its transverse component can take n discrete values, $p_\varphi = s\Delta p_\varphi = \pi\sqrt{3}s/an$ $(s = 1\ldots, n)$. Unlike transverse quasimomentum $p_\varphi(p_\varphi)$, the axial quasimomentum p_z is assumed to vary continuously within the range $0 \le p_z \le 2\pi/a$, which corresponds to the model of infinitely long CNT ($L = \infty$). This model is applicable to the case under consideration because of the restriction to the temperatures and/or voltages well above the level spacing [3], i.e. $k_BT > \varepsilon_C$, $\Delta\varepsilon k_BT > \varepsilon_C$, $\Delta\varepsilon$, where k_B is the Boltzmann constant, T is the temperature, ε_C is the charging energy. The energy level spacing $\Delta\varepsilon$ is given by $\Delta\varepsilon = \pi\hbar v_F/L$, where v_F is the Fermi velocity and L is the carbon nanotube length [3].

We employ the Boltzmann equation with a single relaxation time approximation and follow the procedure of Mensah et al. [26],

$$\frac{\partial f(p)}{\partial t} + eE(t)\frac{\partial f(p)}{\partial P} = -\frac{[f(p) - f_0(p)]}{\tau} \quad (3)$$

where e is the electron charge, $f_0(p)$ is the equilibrium distribution function, $f(p,t)$ is the distribution function at any time (t), and τ is the relaxation time. The electric field $E(t)$ is applied along the CNT axis. The relaxation term, is assumed to be constant and describes the effects of the dominant type of scattering (e.g. electron-phonon and electron-twistons) [3]. Expanding the distribution functions, $f_0(p)$ and $f(p,t)$ in Fourier series,

$$f_0(p) = \Delta p_\varphi \sum_{s=1}^{n} \delta\left(p_\varphi - s\Delta p_\varphi\right) \sum_{r\neq 0} f_{rs} e^{iarp_z} \quad (4)$$

and

$$f(p,t) = \Delta p_\varphi \sum_{s=1}^{n} \delta\left(p_\varphi - s\Delta p_\varphi\right) \sum_{r\neq 0} f_{rs} e^{iarp_z} \varnothing_v(t) \quad (5)$$

where $\delta(x)$ is the Dirac delta function, f_{rs} is the coefficient of the Fourier series and $\varnothing_v(t)$ is the factor by which the Fourier transform of the nonequilibrium distribution function differs from its equilibrium distribution counterpart. The equilibrium distribution function $f_0(p)$ can be expanded in the analogous series with coefficients as follows:

$$f_{rs} = \frac{a}{2\pi} \int_0^{\frac{2\pi}{a}} \frac{e^{-iarp_z}}{1 + \exp\left(\varepsilon_s(p_z)/k_BT\right)} dp_z. \quad (6)$$

Substituting equations (4) and (5) into (3), and solving with equation (1) we obtain:

$$\begin{aligned}\varnothing_v(t) = &\sum_{k_1,k_2=-\infty}^{\infty} \sum_{v_1,v_2=-\infty}^{\infty} J_{k_1}(r\beta_1) J_{k_2}(r\beta_2)\\ &\times J_{k_1+v_1}(r\beta_1) J_{k_2+v_2}(r\beta_2)\\ &\times \left(\frac{(1 - i(k_1\omega_1 + k_2\omega_2)\tau)}{1 + ((k_1\omega_1 + k_2\omega_2)\tau)^2}\right)\\ &\times \left\{\cos\left(v_1\omega_1 t + v_2(\omega_2 t + \theta)\right)\right.\\ &\left. - i\sin\left(v_1\omega_1 t + v_2(\omega_2 t + \theta)\right)\right\} \quad (7)\end{aligned}$$

where $\hbar = 1$, $\beta_1 = eaE_1/\omega_1$, $\beta_2 = eaE_2/\omega_2$ and $J_k(\beta)$ is the Bessel function of the kth order. We determine the surface current density as:

$$j_z = \frac{2e}{(2\pi\hbar)^2} \iint f(p,t) v_z(p)\, d^2p,$$

or

$$j_z = \frac{2e}{(2\pi\hbar)^2} \sum_{s=1}^{n} \int_0^{\frac{2\pi}{a}} f\left(p_z, s\Delta p_\varphi, \varnothing_v(t)\right) v_z\left(p_z, s\Delta p_\varphi\right) dp_z. \quad (8)$$

The integration is taken over the first Brillouin zone. We consider the relation $v_z(p_z, s\Delta p_\varphi) = \partial\varepsilon_z/p_z$ and represent $\varepsilon_z(p_z)/\gamma_0$ by Fourier series with coefficients ε_{rs} defined similarly as in equation (6). Then, substituting equations (5) and (7) into (8) and linearizing with respect to E_2 using $J_{\pm 1}(\beta_2) \approx \pm\beta_2/2$, $J_0(\beta_2) \approx 1 - \left(\beta_2^2/4\right)$ and then

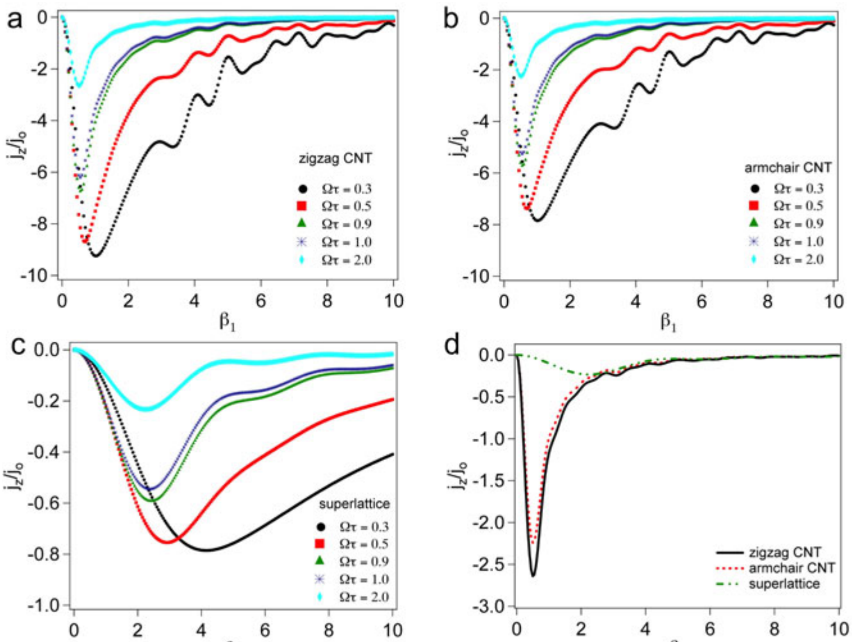

Fig. 1. j_z/j_0 vs. β_1 for $\Omega\tau = 0.3$ (●), $\Omega\tau = 0.5$ (■), $\Omega\tau = 0.9$ (▲), $\Omega\tau = 1.0$ (∗) and $\Omega\tau = 2.0$ (♦) for (a) a zigzag CNT, (b) an armchair CNT and (c) superlattice [20,21]. (d) A comparison of j_z/j_0 vs. β_1 for $\Omega\tau = 2$ for a zigzag CNT (——), an armchair CNT (———) and superlattice (— - —).

averaging the result with respect to time t, we obtain the dc due to $\omega_1 = \Omega$ and $\omega_2 = 2\Omega$ as follows,

$$j_z = \frac{2e^2\gamma_0 a}{\sqrt{3}\hbar n b} E_2 \cos\theta \sum_{r=1}^{\infty} r^2 \times \sum_{k=-\infty}^{\infty} \frac{kJ_k(r\beta_1)\, J_{k-2}(r\beta_1)}{1+(k\Omega\tau)^2} \sum_{s=1}^{n} f_{rs}\varepsilon_{rs}. \quad (9)$$

Superlattices are characterized by the dispersion law $\varepsilon(p) = \frac{\Delta}{2}\left[1-\cos\left(\frac{pd}{\hbar}\right)\right]$, with Δ as the band width, p is the momentum of the electron along the SLs axis, d is the spatial period of the SLs and $\hbar$ is the Planck's constant. Applying the above method to this dispersion law, we obtained the expression,

$$j_z = \sigma_0 E_2 \cos\theta \sum_{k=-\infty}^{\infty} \frac{kJ_k(\beta_1)\, J_{k-2}(\beta_1)}{1+(k\Omega\tau)^2}. \quad (10)$$

Comparing (9) and (10), it is evident that the behavior of the dc of the CNTs is strongly influenced by the presence of the high stark components (i.e., the summation over r) and the specific dispersion law inherent in the hexagonal crystalline structure that make the CNTs highly nonlinear.

3 Results, discussion and conclusion

We discuss the sinusoidal rectification by CNTs subjected to an electric field with two frequencies $\omega_1 = \Omega$ and $\omega_2 = 2\Omega$ using the solution to the Boltzmann's transport equation (9). In Figure 1 we show the graphs of the normalized current density (j_z/j_0) as a function of β_1 $(\beta_1 = eaE_1/\omega_1)$ for $z_c = (\Omega_\tau) = 0.3$, 0.5, 0.9, 1.0 and 2.0 for a zigzag CNT (Fig. 1a), an armchair CNT (Fig. 1b) and a SL (Fig. 1c). First, we discuss the lower region of β_1. As β_1 increases, the normalized current density (j_z/j_0) decreases and reaches a minimum value at the critical amplitude, $\beta_1^{\min}$. Further increase in β_1 beyond the critical amplitude increases the current density. The $\beta_1^{\min}$ and the peak intensity decrease simultaneously with increasing z_c (i.e., increasing Ω). This is observed in all three cases: the zigzag CNT (Fig. 1a), the armchair CNT (Fig. 1b) and the superlattice (Fig. 1c).

Second, the behavior of the normalized current density for the superlattice (Fig. 1c) is monotonic for all z_c values: $z_c = 0.3$, 0.5, 0.9, 1.0 and 2.0. Such monotonic behavior is a characteristic of rectification. However, the normalized current density versus β_1 of the CNTs exhibits oscillations upon increasing β_1 beyond $\beta_1^{\min}$ (Figs. 1a and 1b). The intensity of the oscillations diminish with increasing z_c (increasing Ω) and almost vanishes at $z_c = 2$. In Figure 1d we compare the normalized current density of the SL to that of the CNTs for $z_c = 2$. It is worth emphasizing two important observations in Figure 1d: (1) the critical amplitude $(\beta_1^{\min})$ of the CNTs occurs earlier in the normalized current density characteristics $(z_c \approx 0.5)$ than that of the SL $(z_c =\approx 2)$, i.e., the frequency is four times smaller in the CNTs than in the SL, and (2) the intensity at $\beta_1^{\min}$ is an order of magnitude higher in the CNTs than in the SL, which is quite substantial. This is attributed to the higher density of states of conduction electrons in the CNTs compared to the SL. Furthermore, the nonlinearity in the CNTs structure is determined by the high stark components (summation with respect to r

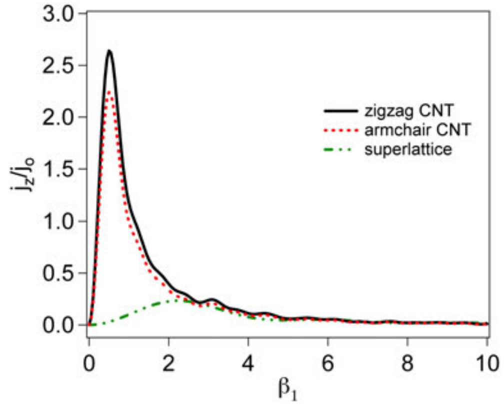

Fig. 2. A plot of j_z/j_0 as a function of β_1 for $z_c = \Omega\tau = 2$ for a zigzag CNT (——), an armchair CNT (- - - - -) and superlattice (— - —) when the phase shift θ lies between $\frac{\pi}{2}$ and $\frac{3\pi}{2}$.

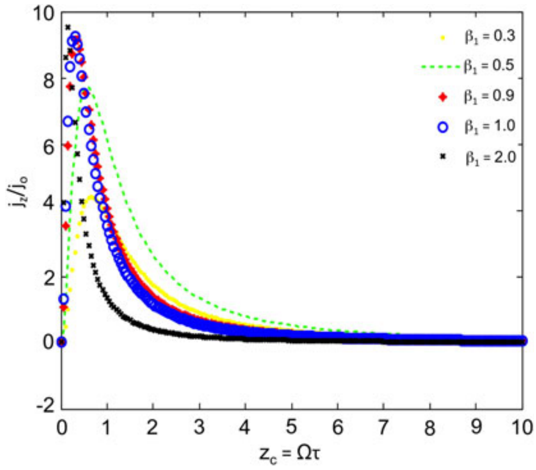

Fig. 3. A comparison of j_z/j_0 versus $\Omega\tau$ for $\beta_1 = 0.3$ (•), $\beta_1 = 0.5$ (- - - -), $\beta_1 = 0.9$ (✚), $\beta_1 = 1.0$ (o) and $\beta_1 = 2.0$ (✖).

in Eq. (9)) and the specific dispersion law inherent in hexagonal crystalline structure. These are absent in the SL (Eq. (10)). We observed an inversion in the current density versus β_1 characteristics when the phase shift θ lies between $\frac{\pi}{2}$ and $\frac{3\pi}{2}$. This is shown in Figure 2 for the zigzag CNT, the armchair CNT and the SL for $z_c = 2$. Shown in Figure 3 is a comparison of a plot of current density (j_z/j_0) as a function of $(\Omega\tau)$ for $\beta_1 = 0.3$, 0.5, 0.9, 1.0 and 2.0. The intensity of the current density increases with increasing β_1, whereas the position decreases with increasing β_1. It is worthwhile to note that $\Omega\tau$ can be used to determine the relaxation time, τ of the electrons in the CNTs. For example, $\tau \approx 1/\Omega$, knowing Ω one can determine τ. On the other hand, for a typical value for τ of 10^{-12} s the frequency $\Omega/2\pi$ would be ~1.5 THz.

In conclusion, we have used the Boltzmann transport equation with constant relaxation time to analyze CNTs and SLs subjected to pure alternating current consisting of two phase-shifted harmonic fields of frequencies $\omega_1 = \Omega$ and $\omega_2 = 2\Omega$ (harmonic mixing), without any dc bias. We observed a direct current generation due to the harmonic mixing. The intensity of the current density is an order of magnitude higher in the CNTs than in the SL and occurred at a frequency one-forth of that of the SL. We attribute these characteristics in CNTs to the high density of states of conduction electrons in carbon nanotubes and the dispersion law of the hexagonal crystalline structure. The rectification is a function of both the frequency and the stark components. Such method could be used to generate terahertz radiation as well as to determine the relaxation time of the carriers in the CNTs.

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