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Terahertz generation and amplification in graphene nanoribbons in multi-frequency electric fields

Rabiu Musah [a,*], Samuel Y. Mensah [b], Sulemana S. Abukari [b]

[a] Department of Applied Physics, Faculty of Applied Sciences, University for Development Studies, Navrongo Campus, Ghana
[b] Department of Physics, Laser and Fiber Optics Center, University of Cape Coast, Cape Coast, Ghana

HIGHLIGHTS

- We used semi-classical transport equations to study THz generation and amplification schemes in monolayer graphene nanoribbons.
- We have studied THz properties of graphene subject to multi-frequency electric fields.
- THz radiations are generated due to amplifications of Bloch oscillation frequencies.
- Amplification in graphene is possible when AC field suppresses electric field domains created by DC field.
- Graphene devices operating at high frequencies in the THz range can be very attractive.

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ABSTRACT

We study theoretically a multi-frequency response of electrons in confined graphene subject to DC–AC driven fields. We explore the possibility for using graphene nanoribbons (GNRs) to generate and amplify terahertz (THz) radiations in electric field domainless regime. We discover two main important schemes of generation; when the frequencies are commensurate, THz generation is due to wave mixing and when they are non-commensurate, a single strong field suppresses space charge instability and any weak signals can get amplified.

1. Introduction

Graphene is a monolayer of one atom thick with fascinating carrier transport properties. Especially, its high carrier mobility of 44,000 $cm^2 V^{-1} s^{-1}$ [1] has attracted a great deal of interests. Attempts to utilize these unique properties in graphene devices are posing some difficulties. The limitation is probably due to several factors including; lack of band gap in graphene sheets, edge defects, disorder, among others. To overcome some of these obstacles, the dimension of graphene sheets can be reduced or the geometry altered. After all, new physics (quantization) emerge when dimensions of materials are reduced. An infinite 2D graphene could become 1D+quantization along one other direction opening a gap. The resulting material is known as graphene nanoribbon (GNR). Depending on the nature of the edges, one can get two symmetry groups from this GNR; armchair graphene nanoribbon (aGNR) or zigzag graphene nanoribbon (zGNR). Electron dynamics of both aGNR and zGNR have different properties, mostly due to the berry phase and pseudospin [2]. Edge states have significant contribution to graphene properties, because in a nanometer size ribbon, massless Dirac fermions can reach the edges within a femto-second before encountering any other lattice effects, like electron–electron interaction, electron–phonon interaction, etc.

In this paper, we study the phenomenon of generation of frequencies in the terahertz (THz) range. The development of sources and sensors emitting and detecting electromagnetic waves in the terahertz regime has been the subject of interest for some time now. And holds great promise for graphene based THz metamaterials, optoelectronic devices, THz lasers, fast switching mechanisms, spectroscopy, wireless communication [3]. Recently, THz generations were studied in graphene using resonance tunneling-like configuration [4] by tunable plasmon excitations, light-plasmon coupling [5] or by optical pumping of graphene

* Corresponding author. Tel.: +233 200916775.
E-mail address: mrabiu@uds.edu.gh (R. Musah).

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[6–8]. Bloch oscillations up to 10 THz can be generated in periodic graphene structures [9]. Today, semiconductor superlattices are used as sources for THz radiation and detection. However, GNRs are better candidates because of their low dimensionality, striking electronic properties and the possibility of controlling these properties via applied gate voltage. Graphene is also relatively easy to fabricate in laboratory.

The physical mechanism governing THz generation in graphene, when subject to applied electric field, can be understood in terms of ballistic trajectories of electrons in the quasi-momentum space. When graphene is subject to an electric field, ballistic acceleration of charge carriers generates to-and-fro motion of the whole distribution function, which varies from zero to several electron volts. It is a collective motion of these charges that manifest THz oscillation of carriers in graphene. The high nonlinearity (non-parabolicity) energy spectrum can also account for THz production in the material. This can be responsible for mismatch between photo electron relaxation and electron–hole recombination rates. The latter effect is more applicable provided frequencies are commensurate. When two or more commensurate frequencies interfere in a region they could result in creation of fields with zero frequencies (static fields). These bias fields are predicted to be responsible for Bloch oscillations at THz frequencies [10].

The remaining of this paper is organized as follows; in Section 2, we introduced the model and theory of the problem. We obtained current density for aGNR and zGNR. By imposing model boundary conditions to reduce the equations to simple forms appropriate for our systems under discussion. Limiting the harmonics fields to only two terms, we deduce *I–V* characteristic equations for describing THz generations in Section 3. The results obtained in the preceding section are analyzed and discussed in Section 4, with conclusions and some recommendations for future work in Section 5.

2. The model and theory

We consider an undoped GNRs (zigzag and armchair) exposed simultaneously to DC+AC electric fields

$$E(t)=E_{DC}+\sum_{j=1}^{n}E_j\ \cos(\omega_j t+\alpha_j). \tag{1}$$

This is seen as a superposition of n harmonic waves polarized along one direction with angular frequencies, ω_i and biased by static field, E_{DC}. The phase difference between the $(j+1)$th and jth component being $\alpha_{j+1}-\alpha_j=\alpha$ is arbitrary, j is an integer. E_j are AC field amplitudes. The dynamics of free $\pi-$electrons in graphene can be describe by the time-dependent Boltzmann transport equation (BTE) based on relaxation time approximation in zero magnetic field as

$$\frac{\partial f(k,t)}{\partial t}+\frac{eE(t)}{\hbar}\frac{\partial f(k,t)}{\partial k}=\Gamma[f(k,t)-f_0(k)], \tag{2}$$

where $f_0(k)$ and $f(t,k)$ are the equilibrium and non-equilibrium Fermi electron distribution functions, respectively. e is the electronic charge, k is the electron wave vector and $\hbar$ is the reduced plank constant. Γ is the reciprocal of the relaxation time, τ.

2.1. Armchair and zigzag nanoribbon band structures

The energy band structure of aGNR and zGNR is characterized by three parameters: band index λ, phase θ and wave vector k [2,11]. For aGNR

$$\varepsilon^{\lambda}(k,\theta)=\lambda\gamma_0\sqrt{1+4\cos^2(s\Delta\theta)+4\ \cos(s\Delta\theta)\cos(kl)} \tag{3}$$

and for zGNR

$$\varepsilon^{\lambda}(k,\theta)=\lambda\gamma_0\sqrt{1+4\cos^2(kl')+4\ \cos(s\Delta\theta)\cos(kl')}, \tag{4}$$

$\lambda=\pm1$; $(+)$ for conduction band and $(-)$ for valence band. $l=\sqrt{3}a/2$, and $l'=a/2$. a is the carbon–carbon distance which has numerical value of 1.42 Å, $\gamma_0\sim3.0$ eV is the overlap integral and θ is the phase perpendicular to the quasi-momentum $\hbar k$. The 1BZ of aGNR is bounded by $kl=[-\pi/2,\pi/2]$ and the zGNR is $kl'=[0,\pi]$. k is parallel to the edge and has translational symmetry along this direction. For aGNR, the transverse wave vector (phase) is quantized according to the rule [2] $\theta_s=s\Delta\theta$ with $\Delta\theta=\pi/(\aleph+1)$ and $s=1,2,\ldots,\aleph$. Unlike aGNR, the nature of transverse wave vector quantization is complicated in zGNR, depending on both \$k\$ and θ as $\Delta\theta_s=(\pi j+\Lambda[k,\theta])/(\aleph+1)$. However, for simplicity we assume Λ is constant, say $\pi/2$, so that $\Delta\theta_s=(j+1/2)\pi/(\aleph+1)$. Except this little subtlety for zGNRs, all that will be discussed in the following for aGNR are equally applied to the zGNR.

Utilizing the translational invariance of the graphene ribbon in the reciprocal space, one can expand in Fourier series functions f, f_0, and ε along the edge having the periodicity in k. i.e.

$$\begin{aligned}f_0(k,\theta)&=\sum_{r\neq0}f_r(\theta)e^{irkl},\ f(k,\theta,t)\\&=\sum_{r\neq0}f_r(\theta)e^{irkl}\Phi_r(t)\ \text{and}\ \varepsilon(k,\theta)=\sum_{r\neq0}\varepsilon_r(\theta)e^{irkl}\end{aligned} \tag{5}$$

The Fourier coefficients f_r and ε_r are expressed as $f_r(\theta)=\sum_{s=1}^{\varkappa}f_{rs}\Delta\theta\delta(\theta_s-s\Delta\theta)$ with $f_{rs}=(l/\pi s\Delta\theta)\int_{-\pi/2l}^{\pi/2l}dkf_0(k,\theta)e^{-irkl}$ and $\varepsilon_r=(l/2\pi\gamma_0)\int_{-\pi/2l}^{\pi/2l}\int dk\,\varepsilon(k)e^{-irkl}$, $f_{rs}=f^*_{-rs}$ and $\varepsilon_r=\varepsilon^*_{-r}$. Subscript s in Eq. (5) counts the number of dimmers $\varkappa$ in GNRs. The factor Φ_r in Eq. (6) is a central point in this paper and so has to be determined. r is an integer and not equal to zero. To compute $\Phi(t)$, Eq. (5) is substituted in Eq. (2) following the simplification scheme j, $j'=1,2,3,\ldots$ and m_j, $n_j=\pm1,\pm2,\pm3,\ldots$. We obtained

$$\Phi_r(t)=\sum_{n_j,\nu_j=-\infty}^{\infty}\prod_{j=1}^{n}J_{n_j}(r\beta_j)J_{n_j-\nu_j}(r\beta_j)\frac{e^{i\nu_j\omega_j t++i\nu_j\alpha_j}}{1+i\tau(r\omega_{DC}+\nu_j\omega_j)}+c.c \tag{6}$$

where $\nu_j=n_j-m_j$, $\beta_j=el\tau E_j/\hbar\omega$ and $\omega_{DC}=elE_{DC}/\hbar$.

2.2. Sheet current density equation

The sheet current density of graphene can be determined from the relation

$$j(t)=\frac{g_s g_v}{4\pi^2}\sum_{s=1}^{\varkappa}\int dk\ v(k,\theta_s)f(k,\theta_s,\Phi_r), \tag{7}$$

where g_s and g_v are the spin and valley degeneracies respectively. The velocity of Dirac fermions in graphene is defined as $v(k)=\partial\varepsilon/\hbar\partial k$. In terms of the Fourier coefficients

$$v(k,\theta)=\frac{i\gamma_0 l}{\hbar}\sum_{r\neq0}r\varepsilon_{rs}e^{irkl} \tag{8}$$

giving

$$j(t)=i\sum_{r=1}^{\infty}j_{DC,r},\Phi_r(t)+c.c, \tag{9}$$

or

$$j(t)=i\sum_{r=1}^{\infty}j_{DC,r}\left[\sum_{n_j,\nu_j=-\infty}^{\infty}\prod_{j=1}^{n}J_{n_j}(r\beta_j)J_{n_j-\nu_j}(r\beta_j)\frac{e^{i\nu_j\omega_j t++i\nu_j\alpha_j}}{1+i\tau(r\omega_{DC}+\nu_j\omega_j)}\right] \tag{10}$$

where the DC current density is

$$j_{DC,r}=\frac{2g_s g_v e\gamma_0}{\pi l\hbar}\Delta\theta\sum_{s=1}^{\varkappa}r\varepsilon_{rs}f_{rs},\ \text{with}\ j^*_{0,r}=-j_{0,-r}$$

and g_s and g_v are the spin and valley degeneracies, respectively.