Amplification of Acoustic Waves in Armchair Graphene Nanoribbon in the Presence of External Electric and Magnetic Field

K. A. Dompreh¹, S. Y. Mensah¹, S. S. Abukari¹, F. Sam¹, and N. G. Mensah²

¹Department of Physics, College of Agriculture and Natural Sciences, U.C.C, Ghana.
²Department of Mathematics, College of Agriculture and Natural Sciences, U.C.C, Ghana

Abstract

Amplification of Acoustic Waves in Armchair Graphene Nanoribbon (AGNR) in the presence of an external Electric and Magnetic field was studied using the quantum kinetic equation. The general expression for the Amplification ($\Gamma_\perp/\Gamma_0$) was obtained in the region $q_l \gg 1$ for the energy dispersion $\varepsilon(\vec{p})$ near the fermi point. For various parameters of the quantized wave vector ($\beta$), the analysis of $\Gamma_\perp/\Gamma_0$ against the sub-bands index ($p_i$), width of AGNR; and magnetic strength ($\phi$), were numerically analysed. The results showed a linear relation for $\Gamma_\perp/\Gamma_0$ with constant electric field ($\vec{E}$) but non-linear for $\Gamma_\perp/\Gamma_0$ with $q$ or $\phi$. Sound Amplification by Stimulated Emission of Radiation (SASER) in AGNR is reported where an increase in Acoustic wave number ($\vec{q}$) causes intraband transition which modulates the Amplification.

Introduction

In low–dimensional materials, particularly Superlattices [1, 2], Quantum Wires [3], and Carbon Nanotubes [4], it is well known that interaction of acoustic phonons with conducting electrons leads to effects such as absorption or amplification of acoustic phonons. In such materials, the study of acoustic wave amplification has attracted much attention due to their use for studying the electronic and other vital properties of thin layers of solids [5]. Graphenes are the latest low-dimensional materials recently discovered [6]. These are single-atom sheet of graphite which shows promising and novel applications in electronic systems. However, charge transport in Graphenes differ from other 2D systems due to lack of an electronic band gap which makes graphenes unsuitable for electronic devices [7]. To overcome this problem, strips of Graphenes called Graphene Nanoribbons (GNRs) whose characteristics are dominated by the nature of their edges are proposed [8, 9]. The Armchair Graphene Nanoribbon (AGNR) and Zigzag Graphene Nanoribbon (ZGNR) with well-defined width
have being extensively studied using the tight-binding approach \cite{10} and Edge-functionalization method in Density Functional Theory (DFT)\cite{11}. The H, -F, -Cl, -Br, -S, -SH and OH are used to engineer the band gap so as to utilise the various properties of GNRs for electronic applications.

In this paper, the quantum kinetic equation for electron-phonon interactions is used to study the Acoustic Wave Amplification in AGNR. This is achieved by applying a sound flux to the AGNR in the presence of external electric and magnetic fields. When the sound flux ($\vec{W}$), electric current ($\vec{j}$) and magnetic field ($\vec{H}$) are mutually perpendicular, the amplification of sound occurs. In this work, it is noted that increasing the acoustic wave number ($\vec{q}$), can lead to intraband transition where Sound Amplification by Stimulated Emission of Radiation (SASER) is seen to occur in AGNR. Varying other parameters such as the sub-band index ($p_i$), the width of AGNR, the energy gap ($E_g$) and the magnetic strength ($\phi$) also modulate the Amplification. This paper is organised as follows: section 1 deals with the introduction; section 2, the theory of the acoustic wave amplification; section 3 is the numerical results and discussions; whilst section 4 is the conclusion.

**Theory**

The general formula for the electronic sound absorption coefficient ($\Gamma_{\vec{q}}$) in the presence of external fields has the form \cite{12}

$$\Gamma(\vec{q}) = \Gamma_0 [1 - \frac{1}{V_s q f_0(\epsilon_0)} \int_\epsilon^\infty \vec{q} f_1(\epsilon) d\epsilon]$$

where $\Gamma_0$ is the absorption coefficient in the absence of external fields, $V_s$ is the speed of sound, $f_0(\epsilon_0)$ is the equilibrium function of the electron distribution and $\vec{q}$ is the wave vector of the sound. The distribution function ($f_{\vec{p}}$) is independent of the acoustic flux, thus

$$f_{\vec{p}} = f_0(\epsilon) + f_1(\epsilon)$$

with $f_1(\epsilon) = \bar{\chi}(\epsilon) \frac{\partial f_0}{\partial \epsilon}$, the $\bar{\chi}(\epsilon)$ characterises the deviation of the distribution function from its equilibrium function and is determined from the Boltzmann kinetic equation. By averaging, Eqn.(1) yields

$$\Gamma(\vec{q}) = \Gamma_0 [1 - \frac{\bar{q} \langle \langle \bar{\chi}(\epsilon) \rangle \rangle}{q V_s}]$$

(3)

The Boltzmann transport kinetic equation is given as

$$- \left( e \vec{E} \frac{\partial f_{\vec{p}}}{\partial \vec{p}} + \Omega [\vec{p}, \vec{H}] \right) \frac{\partial f_{\vec{p}}}{\partial \vec{p}} = - \frac{f_{\vec{p}} - f_0(\epsilon_{\vec{p}})}{\tau(\epsilon_{\vec{p}})} + \pi \xi^2 \bar{W} \frac{\rho V^2_s}{\rho V^2_s} \left\{ [f_{\vec{p}+\vec{q}} - f_{\vec{p}}] \delta(\epsilon_{\vec{p}+\vec{q}} - \epsilon_{\vec{p}} - \omega_{\vec{q}}) + [f_{\vec{p}-\vec{q}} - f_{\vec{p}}] \delta(\epsilon_{\vec{p}-\vec{q}} - \epsilon_{\vec{p}} + \omega_{\vec{q}}) \right\}$$

(4)

where $\vec{E}$ is the constant electric field produced by the acoustic wave in the open-circuited field, $\omega_{\vec{q}} = q V_s$, $\bar{W}$ is the density of the acoustic flux, and $\vec{p}$ the characteristic quasi-momentum of the electron. The relaxation time on energy
where the energy gap $E_g = 3ta_{c-\beta}$ with $\beta$ being the quantized wave vector, $p_i$ the subband index, and $N$ being the number of dimmer lines which determine the width of the GNR. Multiplying the Eqn.(4) by $\vec{p}\delta(\varepsilon - \varepsilon_\vec{p})$ and summing over $\vec{p}$ gives the quantum kinetic equation as

$$\frac{\bar{\vec{R}}(\varepsilon)}{\tau(\varepsilon)} + \Omega[\bar{\vec{R}}, \bar{\vec{R}}(\varepsilon)] = \bar{\Lambda}(\varepsilon) + \bar{\vec{S}}(\varepsilon)$$

(6)

where

$$\bar{\vec{R}}(\varepsilon) \equiv \epsilon \sum_{\vec{p}} \bar{p} f_\vec{p} \delta(\varepsilon - \varepsilon_\vec{p})$$

(7)

$$\bar{\Lambda}(\varepsilon) = -\epsilon \sum_{\vec{p}} \left[ \bar{E}, \frac{\partial f_\vec{p}}{\partial \varepsilon} \right] \bar{p} \delta(\varepsilon - \varepsilon_\vec{p})$$

(8)

$$\bar{\vec{S}}(\varepsilon) = \frac{\pi^2 \bar{W}}{\rho V^2_\beta} \delta(\varepsilon - \varepsilon_\vec{p}) \left\{ [f_{\vec{p}+\vec{q}} - f_{\vec{p}}] \delta(\varepsilon_{\vec{p}+\vec{q}} - \varepsilon_{\vec{p}} - \omega_{\vec{q}}) + [f_{\vec{p}-\vec{q}} - f_{\vec{p}}] \delta(\varepsilon_{\vec{p}-\vec{q}} - \varepsilon_{\vec{p}} + \omega_{\vec{q}}) \right\}$$

(9)

In the linear approximation of $\bar{W}$, $f_\vec{p} \to f_0(\varepsilon_\vec{p})$ with $\vec{p} \to -\vec{p}$, $f_\vec{p} \equiv f_0(\varepsilon_\vec{p}) = f_0(\varepsilon_{\vec{p}})$, Eqns.(8) and (9) expresses to

$$\bar{\Lambda}(\varepsilon) = \bar{E} \left( \frac{2\hbar^2 \beta^2}{\hbar q} - \frac{\hbar q}{2} \right) \frac{\partial f_0}{\partial \varepsilon} \delta(\varepsilon - \varepsilon_\vec{p})$$

(10)

$$\bar{\vec{S}}(\varepsilon) = \frac{2\pi \bar{W}}{\rho V^2_\alpha} \Gamma_0 \left( \frac{2\hbar^2 \beta^2}{\hbar q} - \frac{\hbar q}{2} \right) \Theta(1 - \alpha^2) \frac{1}{\sqrt{1 - \alpha^2}} \frac{\partial f_0}{\partial \varepsilon} \delta(\varepsilon - \varepsilon_\vec{p})$$

(11)

where $\alpha = \frac{\hbar \omega_{\vec{p}}}{\hbar q}$, $\Gamma_0 = \frac{E^2 \alpha^2}{2V^2} f_0(\varepsilon)$ and $\Theta$ is the Heaviside step function where

$$\Theta(1 - \alpha^2) = \begin{cases} 1 & \text{if } (1 - \alpha^2) > 0 \\ 0 & \text{if } (1 - \alpha^2) < 0 \end{cases}$$

Substituting Eqn.(10) and (11) into Eqn.(6) and solving for $\bar{\vec{R}}(\varepsilon)$ gives

$$\bar{\vec{R}}(\varepsilon) = \frac{2\pi \bar{W}}{\rho V^2_\alpha} \Gamma_0 \left( \frac{2\hbar^2 \beta^2}{\hbar q} - \frac{\hbar q}{2} \right) \Theta(1 - \alpha^2) \frac{1}{\sqrt{1 - \alpha^2}} \frac{\partial f_0}{\partial \varepsilon} \delta(\varepsilon - \varepsilon_\vec{p})$$

$$\left\{ \bar{W} \tau(\varepsilon) + \bar{\Omega} \bar{[\bar{E}, \bar{W}]} \tau^2(\varepsilon) + \Omega^2 \bar{[\bar{H}, \bar{W}]} \tau^3(\varepsilon) \right\} + \left( \frac{2\hbar^2 \beta^2}{\hbar q} - \frac{\hbar q}{2} \right) \frac{\partial f_0}{\partial \varepsilon}$$

$$\left\{ \bar{E} \tau(\varepsilon) + \Omega \bar{[\bar{E}, \bar{E}]} \tau^2(\varepsilon) + \Omega^2 \tau^2 \bar{[\bar{H}, \bar{E}]} \right\} \{1 + \Omega^2 \tau^2(\varepsilon)\}^{-1} \delta(\varepsilon - \varepsilon_\vec{p})$$

(12)
Eqn. (12) can be written as \( \vec{R}(\varepsilon) = \vec{\chi}(\varepsilon) \frac{\partial f_0}{\partial \varepsilon} \). In a degenerate system [3],
\[
f_0(\varepsilon_p) = \delta(\varepsilon - \varepsilon_p) = \begin{cases} 0 & \text{if } \varepsilon_p > \varepsilon \\ 1 & \text{if } \varepsilon_p \leq \varepsilon \end{cases}
\]
Where \( \varepsilon \) is the Fermi energy and \( \varepsilon_p \) is given in Eqn. (5). Considering \( \varepsilon_p \leq \varepsilon \) and \((1 - \alpha^2) < 0\), for arbitrary orientation of fields, the \( \vec{\chi}(\varepsilon) \) yields
\[
\vec{\chi}(\varepsilon) = \{\vec{E} \tau(\varepsilon) + \Omega [\vec{h}, \vec{E}] \tau^2(\varepsilon) + \Omega^2 \vec{h}^2(\vec{h}, \vec{E}) \tau^3(\varepsilon)\} \left(\frac{2\hbar^2 \beta^2}{\hbar q - \frac{\hbar q}{2}}\right) \{1 + \Omega^2 \tau^2(\varepsilon)\}^{-1}
\]
(13)
From Eqn. (2), \( f_1(\varepsilon) = \vec{\chi}(\varepsilon) \frac{\partial f_0}{\partial \varepsilon} \) and the current density is given as \( \vec{j} = -\int_0^\infty \vec{R}(\varepsilon) d\varepsilon \) [14]. Ignoring term \( \Omega^2 \vec{h}(\vec{h}, \vec{E}) \tau^3(\varepsilon) \) in Eqn. (13) and averaging over energy, the current density yields
\[
\vec{j} = \{ \langle \tau(\varepsilon) \rangle \vec{E}_y - \langle \frac{\tau^2(\varepsilon)}{1 + \Omega^2 \tau^2(\varepsilon)} \rangle [\Omega, \vec{E}]_y \}
\]
(14)
In Eqn. (14) the following averages were used
\[
\langle (\ldots) \rangle = -\frac{2\pi}{f_0(\varepsilon)} \int_0^\infty (\ldots) \frac{\partial f_0}{\partial \varepsilon} d\varepsilon
\]
\[
\langle \ldots \rangle = -\int_0^\infty (\ldots) \frac{\partial f_0}{\partial \varepsilon} d\varepsilon
\]
Solving for \( \vec{E}_y \) in Eqn. (14) in an open circuit system \( \langle \vec{j}_y \rangle = 0 \), and substituting into Eqn. (13) for \( \langle \langle \vec{\chi}(\varepsilon) \rangle \rangle_\gamma \) gives
\[
\langle \langle \vec{\chi}(\varepsilon) \rangle \rangle_\gamma = \left[ \langle \frac{\tau(\varepsilon)}{1 + \Omega^2 \tau^2(\varepsilon)} \rangle \right] \left(\frac{\tau^2(\varepsilon)}{1 + \Omega^2 \tau^2(\varepsilon)}\right) - \langle \langle \frac{\tau^2(\varepsilon)}{1 + \Omega^2 \tau^2(\varepsilon)} \rangle \rangle \right)
\]
(15)
Inserting Eqn. (15) into Eqn. (3) gives the sound amplification \( \Gamma_\perp \) perpendicular to the electric current \( \langle \vec{j} \rangle \) as
\[
\Gamma_\perp = \Gamma_0 \{1 - \frac{\Omega E_x^2}{V_s} [\langle \frac{\tau(\varepsilon)}{1 + \Omega^2 \tau^2(\varepsilon)} \rangle] \left(\frac{\tau^2(\varepsilon)}{1 + \Omega^2 \tau^2(\varepsilon)}\right) - \langle \langle \frac{\tau^2(\varepsilon)}{1 + \Omega^2 \tau^2(\varepsilon)} \rangle \rangle \}
\]
(16)
Results
The final equation for AGNR in the presence an external magnetic and electric fields is simplified as
\[
\Gamma_\perp / \Gamma_0 = \left[1 - \frac{9\pi^2}{8V_s} \Omega E_x \tau^2 exp(\phi^2) \left\{ \frac{3\pi F_{(-3/2,\phi^2)} F_{(-1/2,\phi^2)}}{F_{(-2,\phi^2)}} - F_{(0,\phi^2)} \right\} \left(\frac{2\hbar^2 \beta^2}{\hbar q - \frac{\hbar q}{2}}\right) \right]
\]
(17)
Figure 1: (a) Dependence of $\Gamma/\Gamma_0$ on $E_0$ for 7-AGNR ($p = 1, 3, 5$), and (b) for $q$ at widths of AGNR = 7, 9, 12.

Figure 2: (a) Dependence of $\Gamma/\Gamma_0$ on the 7-AGNR energy gap ($E_g$) at $p_i = 1, 2, 3$ (b) $\phi$ for the width of AGNR = 7, 9, 12.

Figure 3: A 3D graph of $\Gamma/\Gamma_0$ on $E_0$ and $q$ for $p = 1$ (a) 7-AGNR at $q = 2.0 \times 10^6 \text{cm}^{-1}$, (b) 7-AGNR, $q = 2.5 \times 10^6 \text{cm}^{-1}$. 


with $\phi = \frac{\sqrt{3}}{2} \Omega \tau$, $F_{m,n} = \int_{0}^{\infty} \frac{x^m}{1 + \phi^2 x^2} dx$, $x = \frac{r}{2\alpha}$ and $\beta = \frac{2\pi}{a_{c}\sqrt{3}} \left( \frac{p_{i}}{N+1} \right) - \frac{2}{3}$.

The parameters used in the numerical calculations are as follows: $\tau = 10^{-12} s$, $\omega_q = 10^{10} s^{-1}$, $V_{s} = 5 \times 10^{3} \text{ms}^{-1}$, $H = 2 \times 10^{3} \text{Am}^{-1}$, $q = 2.23 \times 10^{6} \text{cm}$. Figure 1a shows the Amplification of the acoustic wave in 7-AGNR by varying the sub-band index $p_{i} = 2, 4, 5$ at specified electric field. The maximum amplification was obtained at $p = 5$ whilst Figure 1b, showed the non-linear relation for different widths of AGNR (7, 9, 12). A graph of $\Gamma/\Gamma_0$ against the Energy gap $E_g$ is presented in Figure 2a. The $\Gamma/\Gamma_0$ varies for values of $E_g$ between 0 and 0.5 for 7-AGNR at $p_{i} = 1, 2, 3$. The graph of the magnetic strength ($\phi$) presented in Figure 2b. From the graph, ($\phi$) steadily to a maximum at 0.92 then decrease again. In 3D representation, the dependance of $\Gamma/\Gamma_0$ on $q$ and $E$ are shown in Figure 3. There is amplification for 7-AGNR at $q = 2.0 \times 10^{6}$ but increasing $q = 2.5 \times 10^{6}$ modulates the graph. Studies of the transitions in sub-band in the AGNR by tight-binding energy dispersions agrees quantitatively to that of acoustic wave amplification using quantum kinetic equation. In tight-binding approximation, the electronic structure of AGNR strongly depends on its width $2$. This is verified by using 7-AGNR and 8-AGNR at $p = 6$ and an energy gap of 0.3eV (see Figure 4). The 8-AGNR is purely absorbing but 7-AGNR is partially amplifying.

Conclusions

The amplification of the acoustic wave in an external electric and magnetic field is studied using quantum kinetic equation for electron-phonon interactions in AGNR. Analytical expressions for the Amplification under different conditions are numerically analysed. The dependence of $\Gamma/\Gamma_0$ on $E_0$ and $q$ are determined at different values of $\phi$, $p_i$ and the width where the maximum value of the magnetic strength occurs at 0.93. That of $\Gamma/\Gamma_0$ against $q$ is also analysed. In particular, when $q$ is increased from $2.0 \times 10^{6}$ to $2.5 \times 10^{6}$, the amplification is modulated. This indicates intraband transition of SASER in AGNR.
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