

## Linewidth of Cyclotron Absorption in Band-Gap Graphene: Relaxation Time Approximation vs. Monte Carlo Method

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(Received 17 November 2014; revised manuscript received 09 March 2015; published online 25 March 2015)

The power of the elliptically polarized electromagnetic radiation absorbed by band-gap graphene in presence of constant magnetic field is calculated. The linewidth of cyclotron absorption is shown to be non-zero even if the scattering is absent. The calculations are performed analytically with the Boltzmann kinetic equation and confirmed numerically with the Monte Carlo method. The dependence of the linewidth of the cyclotron absorption on temperature applicable for a band-gap graphene in the absence of collisions is determined analytically.

**Keywords:** Graphene, Cyclotron resonance, Monte Carlo method.

PACS numbers: 72.80.Vp, 72.20.Ht, 72.15.Gd

### 1. INTRODUCTION

The possibilities of using of graphene structures in optoelectronics explain the high interest among researchers in studying of non-linear electromagnetic (EM) response of such materials [1-12]. Investigations of magnetic field effect on the kinetics properties of graphene give the information about effective mass, concentration and mobility of charge carriers of graphene structures [1, 13, 14]. The effect of magnetic field on the dc-conductivity of graphene was studied in Refs. [15-17]. The influence of high-frequency radiation on the Shubnikov-de Haas oscillations in graphene was investigated in Ref. [18].

The adequacy of relaxation time approximation ( $\tau$ -approximation) for quasiclassical describing the magnetotransport in graphene was shown in Ref. [17] in the numerical experiment. The simulation performed in Ref. [17] used the Monte-Carlo method taking into account the scattering processes on the acoustic and optical phonons.

Investigations of cyclotron resonance are also important for diagnostic of kinetic properties of 2D-electron systems [19]. In Refs. [20-27] the magneto-optical conductivity of graphene and its cyclotron response were investigated within the linear response theory. The theory of magneto-optical conductivity of graphene taking into account the electron-phonon coupling was developed in Ref. [25]. In Ref. [27] the temperature dependence of high-frequency magnetoconductivity of gapless graphene was calculated. For non-quantizing magnetic field the calculations in Ref. [27] were based on the Boltzmann equation which was written in  $\tau$ -approximation and in linear approximation over the electric field intensity  $\mathbf{E}$ .

Experimental results on the cyclotron resonance in single-layered graphene were published in Refs. [14, 28-30], where the linewidth of the cyclotron reso-

nance was shown to be very broad even in a perfectly pure graphene. This fact was discussed theoretically in Ref. [31] where linear response theory of cyclotron absorption was shown to be not applicable for describing the EM response of gapless graphene in finite magnetic fields.

In Ref. [31] the analysis of equation of motion of single electron with linear dispersion in constant magnetic field with intensity  $\mathbf{H} \neq 0$  and in sinusoidal electric field was performed. The scattering processes were neglected in Ref. [31]. Such situation corresponds to the electron motion in gapless pure graphene. The calculations showed that EM response of gapless graphene was essentially nonlinear even in a weak external electric field ( $E \ll H v_F / c$ ,  $v_F$  is the velocity on the Fermi surface). Mathematically, this result was the consequence of singularity of Lorentz-force term in the equation of motion in the case of non-zero magnetic field. According Ref. [31] the width of cyclotron line has a non-zero width even if all scattering processes are neglected. This fact differs graphene from 2D-systems with parabolic dispersion law [19]. As follows from result of Ref. [31] the non-zero width of cyclotron line is not necessarily related to scattering processes but is due to the linear dispersion of graphene.

Analysis of equation of motion of number electrons in non-zero magnetic field with intensity  $\mathbf{H} \neq 0$  was performed in Ref. [31] also (48 particles). However in a real graphene system one deals with macroscopic ensemble of electrons with different initial phases and initial momenta. Hence the theory must be based on the kinetic equation taking into account scattering processes and the action of EM fields on the electron subsystem as whole. Moreover, according to the theory of transport phenomena [32, 33], the presence of the band gap in graphene leads to the next situation. Firstly if  $\tau$  and gap semiwidth  $\Delta$  satisfy the next inequality:  $e v_F E \tau \ll \Delta$ , then the electron dynamics can be consid-

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ered as linear. Secondly, as will be shown below, for band-gap graphene linear response theory also shows the non-zero width of cyclotron line if scattering frequency  $\nu = \tau^{-1}$  decreases to zero (although, in contradistinction to Refs. [27, 31], the Lorentz-force term in the equation of motion is not singular at low electric fields). Note that the possibility of gap appearance in band structure of graphene was investigated in Refs. [2, 3].

## 2. LINEWIDTH OF CYCLOTRON ABSORPTION OF EM RADIATION BY BAND-GAP GRAPHENE

Let the graphene layer is located on the substrate (SiC or h-BN, for instance). Intensity of magnetic field  $\mathbf{H}$  is orthogonal to the graphene plane  $xy$  which is subjected by the EM radiation polarized elliptically so that intensity of the ac-electric field  $\mathbf{E}$  oscillates in the plane  $xy$  with frequency  $\omega$ :  $\mathbf{E} = E_0 \{ \cos \omega t, \cos(\omega t - \phi) \}$ . The presence of the substrate leads to a gap arising in the electronic spectrum of graphene [2, 3]:

$$\varepsilon(p) = \sqrt{\Delta^2 + v_F^2 p^2}. \quad (1)$$

where  $\Delta$  is the semiwidth of gap in the band structure of graphene.

For electron with momentum  $p_1$  which is in the field of EM wave of frequency  $\omega$  the condition of cyclotron resonance is  $\omega_c(p_1) = \omega$ . If we deal with ensemble of electrons with different momenta the EM energy is absorbed most intensively by those electrons which momenta locate near the magnitude  $p_1$ . Thus for graphene the linewidth of cyclotron absorption  $\delta H$  can be rated with the formula:  $\delta H \sim c\omega\delta\varepsilon(p_1)/e v_F^2$ . Here  $\delta\varepsilon = \delta\varepsilon_\tau + \delta\varepsilon_T$  is energy uncertainty,  $\delta\varepsilon_\tau \sim \hbar/\tau$  is energy uncertainty related with the scattering processes,  $\delta\varepsilon_T \sim T$  is energy broadening related with the thermal

distribution at finite temperature  $T$ . So we have:

$$\delta H \sim \frac{c\omega}{e v_F^2} \left( \frac{\hbar}{\tau} + T \right). \quad (2)$$

It is seen from (2) that linewidth of cyclotron absorption  $\delta H$  is not zero even if the scattering processes are absent:  $\tau = \infty$ .

Now we turn to the quantitative study. The power absorbed by the unit of graphene surface is calculated with the formula:  $Q = \langle \mathbf{j} \cdot \mathbf{E} \rangle$ , where averaging is taken over the period of the oscillations of the vector  $\mathbf{E}$ . The quasiclassical approach based on the Boltzmann kinetic equation gives the next formula for current density  $\mathbf{j}$  aroused under the action of pointed fields:

$$\mathbf{j}(t) = -\frac{e}{\tau} \int_{-\infty}^t e^{-\frac{t-t'}{\tau}} \sum_{\mathbf{p}} \mathbf{v}(\mathbf{p}) f_0(\mathbf{p}_0(\mathbf{p}, t, t')) dt', \quad (3)$$

where  $\mathbf{v} = \partial_{\mathbf{p}} \varepsilon$  is the charge carriers velocity,  $f_0(\mathbf{p})$  is the equilibrium state function, momentum  $\mathbf{p}(t)$  is the solution of the classical equation of motion of charged carrier in the EM field with the initial condition:  $\mathbf{p}(t') = \mathbf{p}_0$ . Linear theory of EM response describes adequately electron dynamics in EM field if graphene has the gap ( $\Delta \neq 0$ ) and the next inequality is performed:  $e v_F E_0 \tau \ll \Delta$ . In this case the solution of equation of motion is found in the linear approximation in variable  $\mathbf{E}$ . As a result we obtain:

$$P(t) = P_0 \exp(i\omega_c(t-t')) + \tilde{P}_+(t) + \tilde{P}_-(t) + \bar{P}_+(t) + \bar{P}_-(t), \quad (4)$$

where

$$\tilde{P}_\pm(t) = \frac{i e E_0 P_0^2 \omega_c e^{i\omega_c(t-t') \mp i\omega t'}}{4\beta_0} \frac{1 - i e^{\pm i\phi}}{\omega_c \mp \omega} \left( \frac{e^{i(\omega_c \mp \omega)(t-t')} - 1}{\omega_c \mp \omega} - i(t-t') \right), \quad (5)$$

$$\bar{P}_\pm(t) = -\frac{i e E_0 e^{\pm i\omega t} (1 + i e^{\mp i\phi})}{2(\omega_c \mp \omega)} \left[ \left( 1 - \frac{|P_0|^2 \omega_c}{2\beta_0 (\omega_c \mp \omega)} \right) \left( 1 - e^{i(\omega_c \mp \omega)(t-t')} \right) - \frac{i |P_0|^2 \omega_c (t-t')}{2\beta_0} e^{i(\omega_c \mp \omega)(t-t')} \right]. \quad (6)$$

Here:  $P = p_x + i p_y$ ,  $P_0 = p_{0x} + i p_{0y}$ ,  $\omega_c = eH\eta_0/c$ ,

$\eta_0 = \eta(p_0)$ ,  $\beta_0 = \beta(p_0)$ ,  $\eta = p^{-1} \partial_p \varepsilon$ ,  $\beta = p^2 \eta (\partial_p^2 \varepsilon - \eta)^{-1}$ .

After substitution (4)-(6) in (3) we derive:  $\mathbf{J} = \mathbf{J}_+ + \mathbf{J}_-$ ,

where  $\mathbf{J} = j_x + i j_y$ ,

$$\mathbf{J}_\pm = \frac{e^2 E_0 \tau e^{\pm i\omega t} (1 + i e^{\mp i\phi})}{2} \sum_{\mathbf{p}_0} \frac{\eta_0 f_0(\mathbf{p}_0)}{1 - i(\omega_c \mp \omega)\tau} \times \left( 1 + \frac{P_0^2}{2\beta_0} \frac{1 \pm i\omega\tau}{1 - i(\omega_c \mp \omega)\tau} \right). \quad (7)$$

Thus the power absorbed by the unit of graphene

surface is:  $Q = Q_+ + Q_-$ , where

$$Q_\pm = \frac{e^2 E_0^2 (1 \pm \sin \phi)}{2\omega} \sum_{\mathbf{p}} \frac{f_0(\mathbf{p}) \omega \tau \eta}{1 + (\omega_c \mp \omega)^2 \tau^2} \times \left( 1 + \frac{P^2}{2\beta} \frac{1 + (\omega^2 - \omega_c^2) \tau^2}{1 + (\omega_c \mp \omega)^2 \tau^2} \right). \quad (8)$$

Quasiclassical approach is applicable for the description of electron motion in magnetic field if Larmor radius much more then de Broglie wavelength:  $\sqrt{\hbar/eH} \gg \lambda_B$ . In graphene for the charge carriers de

Broglie wavelength has the order [14]:  $\lambda_B \sim \hbar v_F / \Delta$ . Substrates SiC and h-BN induce the band gap whose semiwidth is equal 0.13 eV and 0.053 eV correspondingly [2, 3]. In this case quasiclassical approach is adequate if magnetic field intensity satisfy the inequality:  $H \ll 20$  T.

Using (1) we define for graphene:  $\eta = v_F^2 / \varepsilon$ ,  $\beta = -\varepsilon^2 / v_F^2$ . Notice that formula for the absorbed power (8) is applicable for all 2D-electron structures whose dispersion laws determined by the absolute value of momentum  $\mathbf{p}$ . For instance, for the semiconductor with parabolic dispersion law formula (8) gives the well known result [34]. For the graphene subjected to the linear polarized EM radiation and for temperatures close to absolute zero formula (8) leads to the result [26, 27]. In the case of constant electric field ( $\omega = 0$ ) the result [17] follows from (7).

If the temperature satisfies the next inequality  $T \gg n_0 \hbar^2 v_F^2 / \Delta$  ( $n_0 = 10^{10} \text{ cm}^{-2}$  is the surface concentration of charge carriers in graphene<sup>4</sup>) then electron gas is nondegenerate. For the numerical values of the parameters  $\Delta$  and  $n_0$  pointed above temperature of nondegenerate gas should satisfy the inequality:  $T \gg 10$  K. In this case the equilibrium state function  $f_0(\varepsilon)$  is the Boltzmann function. So we have:

$$Q_{\pm} = \frac{\Delta^2 Q_0}{T(T+\Delta)} \int_1^{\infty} \frac{\omega \tau}{z^2 + (\Omega_c \mp \omega z)^2 \tau^2} \times \left( 1 - \frac{z^2 - 1}{2z^2} \frac{z^2 - (\Omega_c^2 - \omega^2 z^2) \tau^2}{z^2 + (\Omega_c \mp \omega z)^2 \tau^2} \right) e^{-\frac{\Delta}{T}(z-1)} z^2 dz \quad (9)$$

where  $Q_0 = e^2 n_0 v_F^2 E_0^2 (1 \pm \sin \phi) / 2\omega \Delta$ .

For definiteness we consider the EM wave polarized circularly ( $\phi = \pi/2$ ). Calculation of the integral in (9) at  $\omega \tau = \infty$  gives:

$$Q = \frac{\pi Q_0}{\omega} \left( \Omega_c + \frac{\Omega_c^2 - \omega^2}{2\Omega_c} \right) \theta(\Omega_c - \omega) e^{-\frac{\Delta}{T} \left( \frac{\Omega_c}{\omega} - 1 \right)}. \quad (10)$$

where  $\theta(x)$  is the step function. Let us introduce the next definition:  $\chi = e v_F^2 \delta H / c \Delta \omega$ , where  $\delta H$  is the cyclotron linewidth. Cyclotron linewidth determined as the deference between magnetic field intensities at which the value of  $Q(H)$  in two times less, than resonance value.

Using formula (10) we find that  $\chi$  is the solution of the next equation:

$$\chi - \frac{T}{\Delta} \ln \left( 3 + 3\chi + \frac{2}{1+\chi} \right) = 0, \quad (11)$$

The solution of (11) is easy to find as the series expansion in powers of  $T/\Delta$ :

$$\delta H = \frac{c \omega T \ln 5}{e v_F^2} \left( 1 + \frac{T}{5\Delta} + \frac{2 + 19 \ln 5}{50} \frac{T^2}{\Delta^2} + \dots \right). \quad (12)$$

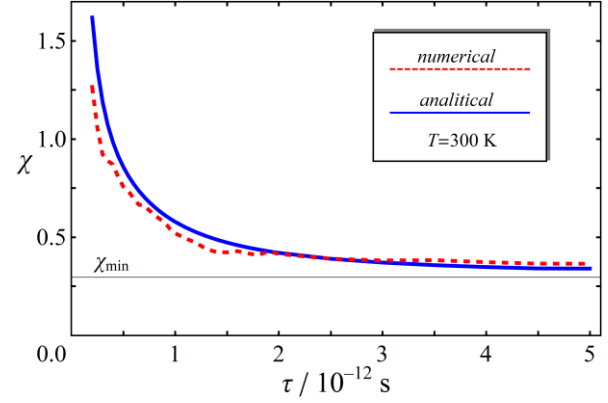


Fig. 1 – Cyclotron linewidth vs. time between collisions

The cyclotron linewidth is seen from (12) is not zero in pure graphene ( $\omega \tau = \infty$ ). In the first-order approximation with respect to the temperature  $T$  result (12) is in agreement with the qualitative estimation (2). Note that formula (12) is obtained for the first time and is applicable only for band-gap graphene and for EM wave with amplitude  $E_0 \ll \Delta / e v_F \tau$ .

### 3. NUMERICAL ANALYSIS OF THE CYCLOTRON ABSORPTION IN BAND-GAP GRAPHENE

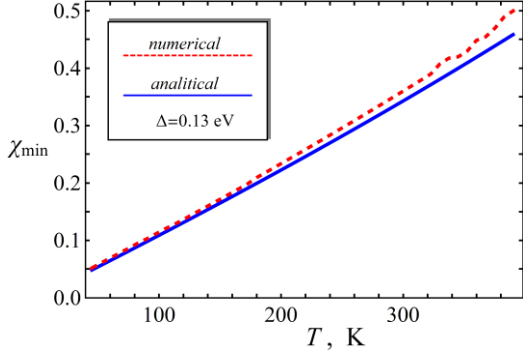
In this section we determine the dependence of EM wave power absorbed by graphene on the magnetic field intensity without using of  $\tau$ -approximation. To this end we use the direct numerical simulation of a Monte Carlo [35, 36]. Charge carriers are supposed to scatter on the phonons (acoustic and optical). Between the acts of scattering the electrons are supposed to move in the magnetic field and in the field of EM wave according to the classical equation of motion. The time  $t_i$  to the  $i$ -th collision is determined from the equation:

$$r = 1 - \exp \left( \int_0^{t_i} W(\mathbf{p}(t')) dt' \right). \quad (13)$$

where  $r$  is a random variable with the uniform distribution in the interval (0, 1),  $W(\mathbf{p})$  is the total scattering probability for an electron with momentum  $\mathbf{p}$ . The duration of a run is divided into small intervals of duration  $\Delta t$ , and the integral in (13) is replaced by the integral sum according to the trapezium method. Next this integral sum, the increment in the electron momentum, and the electron displacement are calculated for each step  $\Delta t$  in a cycle until the following condition is valid:

$$-\ln(r) \leq \frac{\Delta t}{2} \sum_i (W(\mathbf{p}_i) + W(\mathbf{p}_{i-1})). \quad (14)$$

The instant  $t_i$  when condition (14) is satisfied for the first time is the collision instant. The numerical value of  $t_i$  is stored for further averaging. Averaged time is necessary for further comparison of the analytical and numerical results. The scattering mechanism is



**Fig. 2** – Cyclotron linewidth of pure band-gap graphene vs. temperature

determined with the help of the random variable  $s$  uniformly distributed in the interval  $(0, 1)$  according to the following rule:

$$\begin{cases} \frac{W_{\text{opt}}(\mathbf{p})}{W_{\text{ac}}(\mathbf{p}) + W_{\text{opt}}(\mathbf{p})} \geq s, \text{ optical phonons;} \\ \frac{W_{\text{opt}}(\mathbf{p})}{W_{\text{ac}}(\mathbf{p}) + W_{\text{opt}}(\mathbf{p})} < s, \text{ acoustic phonons,} \end{cases} \quad (15)$$

where  $W_{\text{ac}}(\mathbf{p})$  and  $W_{\text{opt}}(\mathbf{p})$  are the probabilities of optical- and acoustic-phonon scattering, correspondingly [17]:

$$W_{\text{ac}}(\mathbf{p}) = \frac{TD_{\text{ac}}^2 \varepsilon(\mathbf{p})}{2\hbar^3 \rho v_s^2 v_F^2}. \quad (16)$$

$$W_{\text{opt}}(\mathbf{p}) = \frac{D_{\text{opt}}^2}{4\hbar^2 \rho \omega_0 v_F^2} \times \begin{cases} \varepsilon(\mathbf{p}) - \hbar\omega_0, & \varepsilon(\mathbf{p}) - \hbar\omega_0 \geq \Delta; \\ 0, & \varepsilon(\mathbf{p}) - \hbar\omega_0 < \Delta, \end{cases} \quad (17)$$

$D_{\text{ac}}$  is the deformation-potential constant,  $\rho$  is the surface density of the material,  $v_s$  is the sound velocity in graphene,  $D_{\text{opt}}$  is the electron-optical phonon interaction constant,  $\omega_0$  is frequency of optical phonon.

As a result, the average value of  $\mathbf{v} \cdot \mathbf{E}$  is calculated. Then the dependence of EM power  $Q$  absorbed by surface unit of graphene on the magnetic field intensity  $H$  and the cyclotron linewidth are found.

In the numerical experiment the next values of parameters are used [37]:  $\rho = 7.7 \times 10^{-8} \text{ g/cm}^2$ ,  $v_s = 10^6 \text{ cm/s}$ ,  $T = 300 \text{ K}$ ,  $\omega_0 = 2.56 \times 10^{14} \text{ s}^{-1}$ . To find the dependence of the cyclotron linewidth on the average time between collisions the constants  $D_{\text{ac}}$ ,  $D_{\text{opt}}$  are changed within the next values 5-30 eV and  $10^{9.5} \times 10^9 \text{ eV/cm}$  correspondingly.

#### 4. DISCUSSIONS

Dependence of linewidth of cyclotron absorption on the relaxation time  $\tau$  is shown in Fig. 1 ( $T = 300 \text{ K}$ , value  $\chi_{\text{min}}$  corresponds to the linewidth expressed in dimensionless units in the absence of collisions). Solid line corresponds to calculation performed in  $\tau$ -approximation. Dashed line corresponds to the numerical simulation with Monte-Carlo method. The cyclotron linewidth is seen from Fig. 1 to differ from zero even in the case even of rare collisions ( $\chi_{\text{min}} \neq 0$ ). The deviation between values of cyclotron width in the absence of collisions ( $\omega\tau \gg 1$ ), which are found by  $\tau$ -approximation and by Monte-Carlo method, is of 5%. Such divergence coincides with error of the numerical calculation approximately. Also deviation of the analytical calculation from the numerical results can be explained by the fact that in theoretical calculation the dependence of the collision frequency on the magnetic field was not taken into account. In the case of constant electric field ( $\omega = 0$ ) the error due to this approximation was shown to be of 5-10% by analysis performed in Ref. [17].

The dependence of cyclotron linewidth  $\delta H$  on the temperature in the absence of collisions is shown in Fig. 2. The solid line corresponds to the analytical calculation (formula (12)). Dashed line corresponds to the numerical simulation. It is seen from Fig. 2 that the behavior of  $\delta H$  with temperature changing obtained analytically in the limit  $\omega\tau = \infty$  is confirmed by numerical experiment also.

Thus the linear response theory based on the kinetic equation was shown above to explain the broadening of cyclotron line  $\delta H$  for band-gap graphene. This broadening is related not only with scattering processes. It is related also with non-parabolic spectrum of graphene (1). The value of linewidth  $\delta H$  of cyclotron absorption is determined not only by the parameter  $\omega\tau$ . Therefore at finite temperature ( $T \neq 0$ ) the Drude formula is not applicable for description the cyclotron resonance in quasiclassical limit. In this case the power absorbed by band-gap graphene is given by the formula (9). At zero-temperature ( $T = 0$ ) formula (9) coincides with Drude formula if the cyclotron mass is considered as the value  $\Delta/v_F^2$ .

#### ACKNOWLEDGEMENTS

The work was supported with the funding of the Ministry of Education and Science of the Russian Federation within the base part of the State task №2014/411 (Project Code: 522).

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