Optical Materials 69 (2017) 328–332

Contents lists available at ScienceDirect

Optical Materials

journal homepage: www.elsevier.com/locate/optmat

Linear and nonlinear magneto-optical absorption coefficients and refractive index changes in graphene

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A R T I C L E I N F O

Article history:
Received 12 March 2017
Received in revised form
11 April 2017
Accepted 23 April 2017

Keywords:
Graphene
Nonlinear magneto-optical properties
Magnetic field

A B S T R A C T

In this work, we study the magneto-optical absorption coefficients (MOACs) and refractive index changes (RICs) in monolayer graphene under a perpendicular magnetic field using the compact density matrix approach. The results are presented as functions of photon energy and external magnetic field. Our results show that there are three groups of the possible transitions: the intra-band, the mixed, and the inter-band transitions; in which the MOACs and the RICs appear as a series of peaks in both intra-band and inter-band transitions between the Landau levels. With an increase magnetic field, the resonant peaks give a blue-shift and reduce in their amplitudes. These results suggest a potential application of monolayer graphene in nanoscale electronic and magneto-optical devices.

1. Introduction

Owning the outstanding transport and optical properties [1–6], graphene has been becoming one of the most attractive candidates for applications in nano-electronic and optoelectronics [7,8]. Because of its appealing physical properties, graphene is also fascinating for basic researches. One of the most of its significant properties comes from the extraordinary Landau levels (LLs) in a perpendicular magnetic field B. The LLs of graphene are not equidistant but proportional to the square root of B, this differs markedly from the normal linear dependence on B in the well-studied case of the conventional two dimensional (2D) systems. Especially, the LL with $n = 0$ is shared by both electrons and holes without any energy gap at all [9]. These marvelous characteristics of graphene's energy spectrum are the cause of its amazing physical properties such as the magneto-optical conductivity [9], the unconventional quantum Hall effect [10–12], the dc conductivity [13], and the phonon-assisted cyclotron resonance [14–16]. Especially, the optical conductivity in graphene has been investigated in both theoretically [17–20] and experimentally [21–23]. Unlike in normal 2D systems, in which only one optical absorption peak is observed centered around the cyclotron energy, in graphene a series of peaks have been demonstrated experimentally [24–26]. Very recently, using broadband terahertz magneto-electro-optical spectroscopy, Poumirol et al. [27] have demonstrated that in graphene both the magnetic circular dichroism and the Faraday rotation can be modulated in intensity, tuned in frequency and, importantly, inverted using only electrostatic doping at a fixed magnetic field.

The agreement between theories and experiments of the optical transport properties of graphene has been demonstrated [28]. After that, the magneto-optical properties have also been studied in some new 2D materials, such as: phosphorene [29], topological

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http://dx.doi.org/10.1016/j.optmat.2017.04.053
0925-3467/

insulator [30], molybdenum disulphide [31,32], WSe_2 [33], silicene [34], and Weyl semimetals [35]. Most of these studies have used the Kubo-type formulas to evaluate the optical conductivity and then to discuss the nonlinear optical properties. In this new work we employ the density-matrix formalism to deal with linear and nonlinear properties in monolayer graphene under perpendicular applied magnetic field. The results are expressed in terms of the absorption coefficients and refractive index changes, which are closer to experimental measurements than the optical conductivity reported in previous studies.

Since the higher confinement effect, the linear and nonlinear properties in low-dimensional systems can be strongly enhanced in comparison with that in bulk semiconductors [36]. Therefore, the linear and nonlinear optical properties of low-dimensional systems have been investigated extensively in recent years. Dakhlaoui [36] has studied the linear and nonlinear optical absorption coefficients (OACs) and RICs between the ground and the first excited states in double quantum wells. Yakar et al. [37] calculated the linear, nonlinear and total OACs of $s \to p$, $p \to d$, and $d \to f$ dipole-allowed transitions between singlet-singlet and triplet-triplet states. Guo et al. [38] investigated the effect of hydrogenic impurity while Shi and Yan [39] studied the polaronic effect on linear and nonlinear OACs and RICs in a quantum dots. Rezaei and Tanhaei [40] have discussed the effects of external fields and geometrical size on the OACs and RICs associated to on-center hydrogenic impurity in a multi-layered spherical quantum dot. The effects of applied electric and magnetic fields on the linear and nonlinear OACs and RICs have also been studied in asymmetric double inverse parabolic quantum well [41], in an asymmetric double quantum well under intense laser field [42], and in finite semi-parabolic quantum dots [43]. However, a detailed investigation of the linear and nonlinear OACs and RICs in graphene in the presence of a quantized magnetic field is still lacking.

In this work, we investigate the linear and nonlinear OACs and RICs in a perpendicular magnetic field, renamed MOACs. Using the density matrix theory, we evaluate the linear and nonlinear MOACs and RICs for transitions between two bands. We investigate MOACs and RICs as functions of the incident photon energy and external magnetic field. The paper is organized as follows: In Sec. 2, we present the theoretical framework; the numerical results and discussion are provided in Sec. 3, and finally, our conclusions are given in Sec. 4.

2. Theoretical framework

We consider a graphene sheet localized in the (xy)-plane under the effects of static magnetic field B, applied in the z-direction. The normalized eigenfunction and the corresponding eigenvalues for a carrier in the Landau gauge for the vector potential $\mathbf{A} = (Bx, 0)$ are written as [44–46].

$$\left|n\right\rangle = C_n e^{-iyx_0/a_c^2}\begin{pmatrix} S_n\phi_{|n|-1}(x-x_0) \\ \phi_{|n|}(x-x_0)\end{pmatrix}, \tag{1}$$

$$E_n = S_n\hbar\omega_c\sqrt{|n|}, \quad n = 0, \pm1, \pm2, \ldots, \tag{2}$$

where the electronic states for a carrier are specified by the set of quantum numbers $\alpha = (n, x_0)$ with n the LL index and $x_0 = k_y a_c^2$ the coordinate of the center of the carrier orbit; $\mathbf{r} = (x, y)$ is the 2D spatial coordinate; $C_n = [(1+\delta_{n,0})/2]^{1/2}$; $a_c = (\hbar/eB)^{1/2}$ is the magnetic length; and $\hbar\omega_c = \gamma\sqrt{2}/a_c$ is the effective magnetic energy with $\gamma = a\gamma_0\sqrt{3}/2$ the band parameter, and a the lattice constant. Besides, $S_n = +1$ and -1 stand for the conduction and valence bands. In Eq. (1), $\phi_{|n|}(x)$ is the normalized harmonic-oscillator function, which is given as

$$\phi_{|n|}(x) = \frac{i^{|n|}}{\sqrt{2^{|n|}|n|!\sqrt{\pi}a_c}} e^{-x^2/2a_c^2} H_{|n|}\left(\frac{x}{a_c}\right), \tag{3}$$

where $H_n(x)$ is the n-th Hermite polynomial.

Using the compact density matrix approach the linear and nonlinear optical absorption coefficients for transitions between two bands $|n\rangle$ and $|n'\rangle$ can be calculated as follows [41,47,48].

$$\alpha^{(1)}(\Omega) = \Omega\sqrt{\frac{\mu}{\varepsilon_r}}\frac{\left|M_{n'n}\right|^2 n_e\hbar\Gamma_0}{(E_{n'n}-\hbar\Omega)^2+(\hbar\Gamma_0)^2} \tag{4}$$

$$\alpha^{(3)}(\Omega, I) = -\Omega\sqrt{\frac{\mu}{\varepsilon_r}}\left(\frac{I}{2\varepsilon_0 n_r c}\right)\frac{\left|M_{n'n}\right|^2 n_e\hbar\Gamma_0}{\left[(E_{n'n}-\hbar\Omega)^2+(\hbar\Gamma_0)^2\right]^2}\left\{4\left|M_{n'n}\right|^2 - \frac{\left|M_{n'n'}-M_{nn}\right|^2\left[3(E_{n'n})^2-4E_{n'n}\hbar\Omega+\hbar^2\left(\Omega-\Gamma_0^2\right)\right]}{(E_{n'n})^2+(\hbar\Omega_0)^2}\right\}, \tag{5}$$

where $\hbar\Omega$ is the incident photon energy, μ is the magnetic permeability, ε_r is the real part of the permittivity, n_e is the carrier density, Γ_0 is the phenomenological relaxation rate, $E_{n'n} = E_{n'} - E_n$ is the energy difference between the two levels, I is the optical intensity of the incident photon which excites the system and leads to the optical transitions, c is the speed of light, ε_0 is the permittivity of free space, and n_r is the refractive index. With the help of Eq. (1), the dipole matrix element, $M_{n'n} = \langle n'|ex|n\rangle$, for x-polarized incident radiation, is calculated as follows

$$M_{n'n} = eC_nC_{n'}S_nS_{n'}\left[x_0\delta_{|n'|,|n|} + \left(a_c\big/\sqrt{2}\right)\left(\sqrt{|n|+1}\,\delta_{|n'|,|n|+1} + \sqrt{|n|}\,\delta_{|n'|,|n|-1}\right)\right]. \tag{6}$$

Thus the total optical absorption coefficients is

$$\alpha(\Omega) = \alpha^{(1)}(\Omega) + \alpha^{(3)}(\Omega, I). \tag{7}$$

The linear and nonlinear relative refractive index change with the incident photon energy $\hbar\Omega$ and the system optical radiation intensity I can be expressed as [36,49].

$$\frac{\Delta n^{(1)}(\Omega)}{n_r} = \frac{n_e\left|M_{n'n}\right|^2}{2n_r^2\varepsilon_0}\left[\frac{E_{n'n}-\hbar\Omega}{(E_{n'n}-\hbar\Omega)^2+(\hbar\Gamma_0)^2}\right], \tag{8}$$

$$\frac{\Delta n^{(3)}(\Omega, I)}{n_r} = -\frac{\mu c\left|M_{n'n}\right|^2}{4n_r^3\varepsilon_0}\frac{n_e I}{\left[(E_{n'n}-\hbar\Omega)^2+(\hbar\Gamma_0)^2\right]} \times \left\{4(E_{n'n}-\hbar\Omega) \times \left|M_{n'n}\right|^2 - \frac{(M_{n'n'}-M_{nn})^2}{(E_{n'n})^2+(\hbar\Gamma_0)^2}\left[(E_{n'n}-\hbar\Omega) \times \left[(E_{n'n})(E_{n'n}-\hbar\Omega)-(\hbar\Gamma_0)^2\right] - (\hbar\Gamma_0)^2(2E_{n'n}-\hbar\Omega)\right]\right\}. \tag{9}$$

Finally, the total relative index change can be written as