Physica E 70 (2015) 28–34

Contents lists available at ScienceDirect

Physica E

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

Anisotropic optical conductivity and electron–hole asymmetry in doped monolayer graphene in the presence of the Rashba coupling

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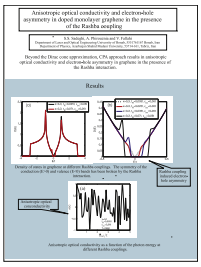
HIGHLIGHTS

- Coherent potential approach in graphene.
- Rashba coupling induced electron–hole symmetry breaking.
- The effect of the impurities on density of states in graphene.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 9 May 2014
Received in revised form
25 November 2014
Accepted 21 January 2015
Available online 20 February 2015

Keywords:
Graphene
Rashba coupling
Optical conductivity
Electron–hole asymmetry
CPA

ABSTRACT

In this study, the optical conductivity of substitutionary doped graphene is investigated in the presence of the Rashba spin orbit coupling (RSOC). Calculations have been performed within the coherent potential approximation (CPA) beyond the Dirac cone approximation. Results of the current study demonstrate that the optical conductivity is increased by increasing the RSOC strength. Meanwhile it was observed that the anisotropy of the band energy results in a considerable anisotropic optical conductivity (AOC) in monolayer graphene. The sign and magnitude of this anisotropic conductivity was shown to be controlled by the external field frequency. It was also shown that the Rashba interaction results in electron–hole asymmetry in monolayer graphene.

1. Introduction

Recently graphene has attracted a rapidly growing interest due to its potential application in nano-electronics [1,2]. The extremely high mobility of graphene, in comparison with conventional semiconductors, constitutes a natural outstanding candidate to design high performance electronic devices for next generation electronics. Due to these surprising features of graphene, the coming years has been named as carbon new age [3]. However lack of an energy gap in graphene is one of the biggest hurdles for graphene device applications [4].

The effect of Spin orbit coupling (SOC) on the monolayer graphene was found firstly by Kane and Mele [5,6]. Strength of intrinsic spin orbit coupling (ISOC) in comparison with the RSOC is very small [7–12]. Meanwhile the RSOC strength in graphene has been reported up to 0.2 eV [13] where can be considered as a really high value for a typical spin–orbit interaction.

The RSOC has been observed by impurity doping and external electric field where the strength of doping induced RSOC is very weak [14]. Meanwhile, it was shown that the RSOC can open and

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http://dx.doi.org/10.1016/j.physe.2015.01.032
1386-9477/

control a noticeable gap at the Dirac points [8,15].

The effect of the RSOC on heavy doped graphene has been investigated in [16]. The effect of the impurities has been considered by choosing chemical potential close to the M point in the first Brillouin zone (BZ) [16]. Results of this research show that the RSOC in mono-layer graphene can strongly affect the optical response of graphene [16].

In the present study we formulated the effect of the impurities on the optical conductivity of the mono-layer graphene in the presence of RSOC. Numerical calculations have been performed under the coherent potential approximation (CPA) where we have shown that the density of states and the transition rate can be effectively controlled by the density of impurities. It was shown that the RSOC removes the electron–hole band symmetry. In this way we have to consider the deformation of the band energies and density of states as a result of the impurities.

Owning to the fact that the RSOC Hamiltonian is translationally invariant, it can be formulated under CPA approach as shown in later sections. The CPA is one of the important and widely used methods for describing disordered systems. The problem is that how conductivity of disordered graphene can be affected by the RSOC under CPA approach?

In this manuscript, band structure of graphene has been studied beyond the Dirac cone approximation in framework of tight-binding Hamiltonian. As a result, trigonal warping (TW) of the energy bands can contribute in optical conductivity. The TW is observed when Fermi circle of a degeneracy point leads to deformation [17] by increasing the Fermi energy. TW was expected to be responsible for anisotropic optical conductivity (AOC) as it removes isotropic band cross sections at Fermi level, however the results of the current study show that, even at low Fermi energies, i.e. when the TW is negligible the amount of the AOC is really significant. Dirac-cone approximation suppresses the TW effect and therefore the intrinsic anisotropy of the bands (regardless of the position of the Fermi energy) can be responsible for AOC of single layer graphene. It seems that the TW could produce some kind of anisotropic effects when, only the occupied states are allowed to contribute in this process. Meanwhile it should be noted that in some of the physical processes such as optical absorption, where a transition is required between an occupied and another empty state. The anisotropy of the entire band energies could result in AOC. The effect of the RSOC on the AOC of a monolayer graphene has also been studied in the current work. The AOC manifests itself when the optical conductivity was different along x and y directions.

Electron density of state (DOS), the optical conductivity of graphene can be controlled by manipulating gate voltage which controls the RSOC strength. Optical properties of a pure monolayer graphene have been studied in [18]. Where it was shown that RSOC can result in a controllable blue shift. In the present work, density of state, AOC of disordered graphene calculated beyond the Dirac-cone approximation.

2. Theoretical model

In the current work we have considered a monolayer graphene, in which its two-dimensional lattice has been oriented with respect to the x- and y-axis as shown in Fig. 1.

Nearest neighbor-tight binding Hamiltonian of pure graphene reads

$$H_0 = -t \sum_{\langle i,j\rangle,\sigma} (a^{\dagger}_{\sigma,i} b_{\sigma,j} + h.c) \tag{1}$$

Where the operators $a^{\dagger}_{\sigma,i}$ and $b_{\sigma,j}$ denote the creation and annihilation of an electron with spin σ in sublattices A and B (Fig. 1),

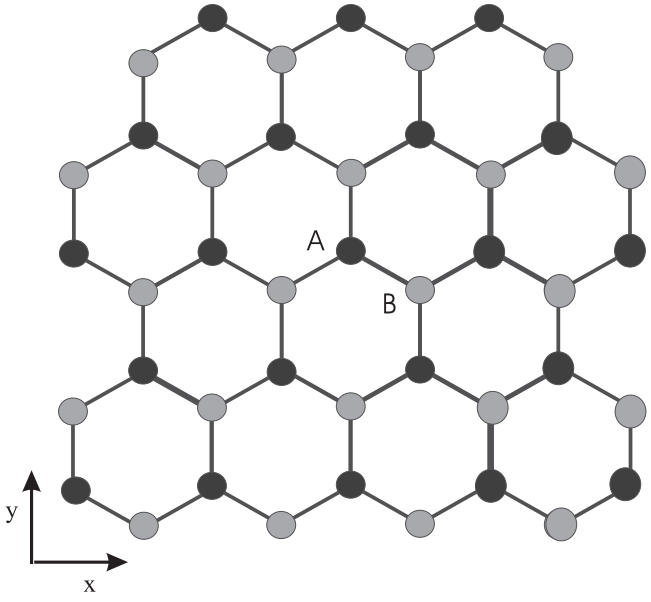

Fig. 1. Spatial orientation of the monolayer graphene with respect to the x- and y-axis and A, B sublattices.

respectively. Where t=2.66 eV is a hopping parameter.

RSOC can generate a gap in graphene and converts graphene to semiconductor. According to the results of density functional theory and other approaches, the strength of the ISOC is several orders of magnitude weaker than the strength of RSOC (the strength of ISOC is about 1–50 μeV) [7–13]. Therefore in this paper the effect of ISOC (also ISOC in next nearest neighbor) is neglected.

RSOC in graphene and other structures emerges when lattice inversion symmetry is broken [19]. In this study RSOC can be considered to be induced by perpendicular gate voltage or by coupling with the substrate. Rashba coupling is given in the form of a nearest neighbor hopping term as follows [14]:

$$H_R = -t_R \sum_{\langle i,j\rangle} c_i^{\dagger}(\mathbf{s}\times \hat{d}_{ij}).\hat{z}c_j + h.c. \tag{2}$$

$\mathbf{s}$ is the vector of Pauli matrices, $\hat{d}_{ij}$ is the unit vector that connects the i and j lattice sites and t_R is the strength of RSOC where $\langle i,j\rangle$ indicates that the sum is performed over the nearest neighbors (Fig. 1) where $c_i^{\dagger}$ (c_i) is the creation (annihilation) operator in one of the A or B sublattices.

Matrix representation of total Hamiltonian on wave function $\psi = (\psi_{A\uparrow}, \psi_{A\downarrow}, \psi_{B\uparrow}, \psi_{B\downarrow})$ is given by

$$H_0 = \begin{pmatrix} 0 & 0 & \gamma(\mathbf{k}) & 0 \\ 0 & 0 & 0 & \gamma(\mathbf{k}) \\ \gamma^*(\mathbf{k}) & 0 & 0 & 0 \\ 0 & \gamma^*(\mathbf{k}) & 0 & 0 \end{pmatrix}, \tag{3}$$

and

$$H_R = \begin{pmatrix} 0 & 0 & 0 & \beta_+(\mathbf{k}) \\ 0 & 0 & \beta_-(\mathbf{k}) & 0 \\ 0 & \beta_-^*(\mathbf{k}) & 0 & 0 \\ \beta_+^*(\mathbf{k}) & 0 & 0 & 0 \end{pmatrix}. \tag{4}$$

where $\gamma(\mathbf{k}) = e^{-iak_y} + 2e^{-i(a/2)k_y}\cos(a_1k_x)$ $\beta_{\pm} = i\,t_R(\xi_1(k) \pm \xi_2(k))$, $\xi_1(k) = e^{ia_1k_x}(e^{-ia_2k_y} - \cos(a_1k_x))$ and $\xi_2(k) = \sqrt{3}\,e^{ia_1k_x}\sin(a_1k_x)$ in which $a_1 = \frac{\sqrt{3}a}{2}$, $a_2 = \frac{3}{2}a$ in which the carbon–carbon distance is denoted by a=1.42 Å.