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Optical conductivity of ABA stacked graphene trilayer: mid-IR resonance due to band nesting

Zeinab Rashidian1,2, Yuliy V Bludov1, Ricardo M Ribeiro1, N M R Peres1 and Mikhail I Vasilevskiy1

1 Centro de Física and Departamento de Física, Universidade do Minho, Campus de Gualtar, Braga
4710-057, Portugal
2 Department of Physics, Faculty of Science, Lorestan university(lu), Lorestan, Iran

E-mail: mikhail@fisica.uminho.pt

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Abstract

The band structure and the optical conductivity of an ABA (Bernal-type) stacked graphene trilayer are calculated. It is shown that, under appropriate doping, a strong resonant peak develops in the optical conductivity, located at the frequency corresponding to approximately 1.4 times the interlayer hopping energy and caused by the ‘nesting’ of two nearly parabolic bands in the electronic spectrum. The intensity of this resonant absorption can be controlled by adjusting the gate voltage. The effect is robust with respect to increasing temperature.

Keywords: graphene, Bernal stacking, optical absorption

(Some figures may appear in colour only in the online journal)

1. Introduction

Since the isolation of monolayer graphene almost a decade ago [1], there has been a high interest in the low energy transport and optical properties of not only the monolayer [2, 3] but also a few layer graphene systems [4–8]. These properties are determined by the electronic band structure near the K point. The undoped monolayer graphene (MLG) is characterized by the universal optical conductivity, \( \sigma_0 = e^2/(4\hbar) \). This implies that the transmittance depends solely on the fine structure constant and originates the quantized visible opacity of suspended monolayer graphene [9, 10]. As far as doped graphene is concerned, there are several effects that arise in the optical properties, related to the restrictions introduced on the interband transitions by the state filling and also to the onset of intraband transitions [11]. The latter correspond to plasmons and give rise to the interesting and promising field of graphene plasmonics [3, 12].

Graphene multilayers offer a new ingredient to the interesting physics and potential applications. The relatively weak interlayer coupling, on the one hand, implies that they should inherit some properties of the parent material [4], on the other hand, it introduces a new energy scale, of the order of few tenths of the electron-volt, that should yield some new properties. It has been shown [13] that there is also a universal optical conductivity in a undoped N-layer graphene, equal to \( \sigma_{0N} = N\sigma_0 \), that is reached in undoped graphene in the low frequency limit. At the same time, the optical response of doped bilayer graphene reveals intense strongly doping-dependent features in the mid-infrared (around 0.4 eV) [5, 6]. The origin of these experimentally observed features has been considered theoretically in these works and also, in more detail, in [14], where the band structure and the optical conductivity of bilayer graphene were calculated. Some novel plasmonic effects in Bernal-stacked bilayer graphene were predicted in the recent work [15]. As the number of layers increases beyond \( N = 2 \), the band structure and the optical conductivity become dependent not only on \( N \) but also upon the stacking arrangement. There are three distinct planar projections of the honeycomb lattice (usually denoted A, B and C) and, consequently, \( 2^{N-2} \) distinct \( N \)-layer sequences [13]. In particular, the stacking of three layers in a graphene trilayer can be either ABA (also called Bernal-type) and ABC (rhombohedral) [16]. These two different stacking arrangements lead to strikingly
different electronic band structures [17]. For instance, it was found that undoped graphene ABC trilayer shows many-body correlations with an energy gap, while the Bernal-type stacking (taking place in graphite) does not lead to a gap [18]. Non-Bernal stacked multiple graphene layers have attracted a considerable attention related to the prospect of further enhancement of capabilities of graphene-based optoelectronic devices, in particular, THz and IR photodiodes [19]. The optical conductivity of ABC trilayers has been considered in a number of works [20–22], in particular, the effect of doping has been analysed [22]. Even though trilayer graphene contains, on average, regions of ABC and ABA stacking in an 15:85 ratio [23], apparently the optoelectronic properties of the latter attracted less attention and we are aware of only one work [24] devoted to this topic. This is notwithstanding the possibility of using far-infrared (FIR) spectroscopy, along with the common Ramon scattering technique [25] in order to distinguish different trilayer graphene species [23, 24].

Therefore, the main purpose of this article is to analyse the spectral characteristics of the optical conductivity of intrinsic and doped ABA stacked trilayers. The mirror-symmetric Bernal stacking is the most common in graphene multilayers and one can expect that the optical conductivity of ABA trilayers can have a monolayer- or bilayer-like character [26]. We shall present the analytical dispersion relation for the electrons near the Dirac point, from which it follows that the band structure of the ABA trilayer indeed looks like a superposition of those characteristic of a monolayer and a bilayer, although the latter corresponds to an effective crystalline structure [7]. Intuitively, one can expect that the density of states of the ABA trilayer is dominated by a narrow resonant peak at the frequency corresponding to this effective interlayer hopping energy (approximately 0.56 eV). It is caused by the fact that the dispersion curves corresponding to two bands are nearly parallel for a considerable range of wavevectors near the Dirac point. This effect sometimes is called ‘band nesting’ [27] in order to distinguish from van Hove singularities in the single-particle density of states. We will show that the intensity of this resonant absorption is approximately proportional to the Fermi energy and, therefore, can be controlled by adjusting the gate voltage applied to the graphene layer.

2. Theoretical background

2.1. Band structure

The tight-binding Hamiltonian for non-interacting electrons in the ABA stacked trilayer involves three A-type and three B-type sites and includes the essential in-plane ($t_0 \approx 2.7$ eV) and interlayer hoppings ($t_1 \approx 0.4$ eV) as shown in figure 1. These two parameters, connecting atoms that are right on top of each other in adjacent layers, are sufficient to describe the main features of the band structure, such as the type of dispersion of the energy bands and their separation, as confirmed by recent DFT calculations [17]. Keeping only $t_0$ and $t_1$ hoppings permits to obtain simple formulae for band gaps, effective masses and the Fermi velocity.

Then the Hamiltonian is given by [18]:

$$
\hat{H} = -t_0 \sum_{n, \delta_j} \langle A_1, \vec{R}_n \rangle \langle \vec{R}_n + \vec{\delta}_j | B_1, \vec{R}_n \rangle - t_0 \sum_{n, \delta_j} \langle A_3, \vec{R}_n \rangle \langle \vec{R}_n + \vec{\delta}_j | B_3, \vec{R}_n \rangle - t_0 \sum_{n, \delta_j} \langle A_2, \vec{R}_n \rangle \langle \vec{R}_n + \vec{\delta}_j | B_2, \vec{R}_n \rangle
$$

$$+ t_1 \sum_n \langle A_2, \vec{R}_n \rangle \langle B_3, \vec{R}_n \rangle + \mathbf{H.c.} \quad (1)
$$

Here $n = (n_1, n_2)$ is the composite index, which determines the atomic positions in the lattice, $\vec{R}_n = n_1 \vec{g}_1 + n_2 \vec{g}_2$, with $\vec{g}_1 = (\sqrt{3}/2, 1/2) a_0$, $\vec{g}_2 = (-\sqrt{3}/2, 1/2) a_0$ being the lattice vectors. The three vectors that connect the B atom to its three nearest neighbors are $\vec{\delta}_1 = (\sqrt{3}, -1/2) a_0$, $\vec{\delta}_2 = (-\sqrt{3}, -1/2) a_0$, and $\vec{\delta}_3 = (0, 1) a_0$, where $a_0$ is the C–C interatomic distance. The positions of the A atoms relative to the B atoms in each of the three layers are shown in figure 1.

The energy spectrum of the Hamiltonian (A.4) is composed of six energy bands given by (see appendix A for details):

$$E_{\pm 1}(\vec{k}) = \pm \sqrt{t_1^2 + |\phi(\vec{k})|^2 - t_1 \sqrt{t_1^2 + 2|\phi(\vec{k})|^2}} \quad (2)
$$

$$E_{\pm 2}(\vec{k}) = \pm |\phi(\vec{k})|^2 \quad (3)
$$

$$E_{\pm 3}(\vec{k}) = \pm \sqrt{t_1^2 + |\phi(\vec{k})|^2 + t_1 \sqrt{t_1^2 + 2|\phi(\vec{k})|^2}} \quad (4)
$$

where

$$\phi(\vec{k}) = -t_0 \left[ \exp(ik_x a_0) + 2 \exp\left(\frac{-ik_x a_0}{2}\right) \cos\left(k_x \sqrt{3} a_0 / 2\right) \right] \quad (5)
$$

The band structure is depicted in figure 2. Note that the gap between the bands $\pm 3$ and the Dirac point is $2D = 2\sqrt{2}t_1$. 