Armenian Journal of Physics, 2019, vol. 12, issue 1, pp. 33-39

Interaction of Electromagnetic Field with Gated Graphene Bilayer

A. P. Djotyan [1], A. A. Avetisyan[1], and K. Moulopoulos[2]

[1]*Yerevan State University, Department of Physics, 1 Alex Manoogian, Yerevan, 0025, Armenia*

[2] *Department of Physics, University of Cyprus, Nicosia, Cyprus*

*E-mail: adjotyan@ysu.am

Received 12 January 2019

Abstract. In this work we investigate the binding energy of excitonic states generated by an electromagnetic field of laser radiation in bilayer graphene with an energy gap opened by perpendicular electric field (by gate voltage). For this purpose we use tight-binding approach and the second quantized Hamiltonian. For Coulomb problem in gapped bilayer, an analytical method based on a variational approach is also suggested. The binding energy of an impurity electron in bilayer graphene is studied by this method and it is shown that the energy is tunable by the gate voltage in the region about ten *meV*.

Keywords: bilayer graphene, electromagnetic field, terahertz radiation, excitonic and impurity states

1. Introduction

The problem of the finding of new and effective sources of terahertz radiation is very important since such devices can be largely used in different fields of science and technology, e.g. in biology, medicine, astronomy, environmental monitoring, and security systems [1]. From this point of view, it is very interesting to investigate the behavior of graphene systems with opened energy gap in electromagnetic field since they can be considered as alternative source of terahertz radiation.

It is well known, that a graphene monolayer is a gapless semimetal with the massless Dirac fermions; the role of the light velocity c here plays the parameter $v_F \approx 10^6 m/\mathrm{s}$, which is smaller by two orders than the light velocity c [2]. On the other hand, a bilayer graphene is a semiconductor that exhibits more intriguing properties: the charge carriers here are chiral quasiparticles with a dominantly parabolic dispersion [3]. It has been predicted that the asymmetry between the on-site energies leads to a tunable gap between the conduction and valence bands [3, 4]. Theoretical and experimental investigations have shown that a perpendicular electric field applied to bilayer of graphene modifies its band structure near the K point and may open an energy gap in the electronic spectrum [5]. Moreover, there is an experimental possibility of controlling the magnitude of the gap and to tune it by the gate voltage. Magnetotransport experiments showed that the induced gap between the conduction and valence bands could be tuned between zero and mid-infrared energies [5]. This makes bilayer graphene the only known semiconductor with a tunable energy gap and may open the way for developing photodetectors and lasers tunable by the electric field effect.

More reach physics is expected for graphene multilayers [6], where the magnitude of the gap strongly depends on the number of graphene layers and its stacking order. In [7, 8] we theoretically studied electric field induced band gap dependence in graphene multilayers on different ways of stacking between consecutive graphene planes. A band structure of multilayer graphene systems required for different aims of nano- and optoelectronics can be theoretically found and suggested for an experimental realization by corresponding choice of the number of layers and by application of electric field of necessary magnitude. In [9], we develop a microscopic theory of a strong electromagnetic field interaction with bilayer graphene systems with an energy gap opened by external gates in the range of 150-250 meV. It was shown that at resonant photon energy close to the energy gap and by adiabatically changing the gate potentials on time, one can produce full inversion of the electron population between valence and conduction bands. For smaller values of the gap, such systems might be useful for the creation of terahertz radiation sources.

One of the most promising mechanisms for generation of terahertz radiation in the far-infrared region is based on optical transitions between the energy levels of shallow impurity centers in semiconductors and semiconductor nanostructures under the impurity breakdown [1,10]. It is interesting to investigate similar phenomena in bilayer as well as in graphene multilayers, where bound states exist for arbitrary weak impurity potential and their binding energies and localization lengths can be changed in a desirable way by changing the gate voltage. Coulomb problem in gapped graphene systems was considered in [11-13].

In this work we study the binding energy of excitonic states in gapped graphene bilayer created by electromagnetic field of laser radiation. We use tight-binding approach and second quantized Hamiltonian and consider only low excitation regime, where a small density of electron hole pairs exists. For better understanding of the influence of band structure parameters on the binding energy we suggest a transparent analytical method based on a variational approach. The plan of the paper is as follow: in Section 2.1 we study the binding energy of excitons created by an electromagnetic field of laser in bilayer graphene with opened energy gap in linear regime. Section 2.2 presents the variational method for an impurity electron in a gapped graphene. Section 3 presents our main results and discussions. Our conclusions are presented in Section 4.

2. Theoretical approaches

2.1. Binding energy of an exciton in a gapped graphene bilayer

The Hamiltonian for bilayer graphene in the vicinity of the *K* point (near the Fermi energy) for the case of two band model has the following form

$$H_0 = \begin{pmatrix} -U/2 & v_3(p_x + ip_y) - (1/2m)(p_x - ip_y)^2 \\ v_3(p_x - ip_y) - (1/2m)(p_x + ip_y)^2 & U/2 \end{pmatrix}, \quad (1)$$

where U is the gap induced by a static perpendicular electrical field, $\mathbf{p}=\{\mathrm{p_x},\mathrm{p_y}\}$ is the electron momentum operator, $v_3=\sqrt{3}\gamma_3 a/2\hbar\approx 0.1\mathrm{v_F}$ is the effective velocity, and $\mathrm{v_F}$ is the Fermi velocity in monolayer graphene (here we omit the real spin and valley quantum numbers), and a is the lattice constant. Tight-binding parameter γ_3 describes the interaction between different *B* atoms in neighboring layers ($\gamma_3\approx 0.31eV$). We use dipole approximation to describe the interaction of an electromagnetic wave with bilayer graphene, and assume that the laser pulse propagates in the perpendicular direction to graphene plane (XY) and the electric field of pulse ***E***(t) lies in the graphene plane.

Introducing $\theta(p)=\arctan(p_y/p_x)$, $p_x+ip_y=p\exp(i\theta)$, the expression for the energy spectrum of bilayer graphene can be presented in the form:

$$\varepsilon_{p,\sigma}=\sigma\sqrt{\frac{U^2}{4}+(v_3 p)^2-\frac{v_3 p^3}{m}\cos 3\theta+(\frac{p^2}{2m})^2}\,, \tag{2}$$

where the index $\sigma=1$ is connected with the conduction band and the index $\sigma=-1$ is related to the valence band. The free solutions in bilayer graphene $\psi_\sigma(\mathbf{p})$ have following form

$$\psi_\sigma(\mathbf{p})=\frac{\sqrt{\varepsilon_{\mathrm{p}\sigma}+U/2}}{\sqrt{2\varepsilon_{\mathrm{p}\sigma}}}\begin{pmatrix}1\\ \dfrac{1}{\varepsilon_{\mathrm{p}\sigma}+U/2}\gamma(p,\theta)\end{pmatrix}, \tag{3}$$

with $\gamma(p,\theta)=-\frac{p^2}{2m}\exp(i2\theta)+v_3 p\exp(-i\theta)$.

In order to investigate excitonic states we use second quantization formalism [9] with the single-particle density matrix in momentum space defined as:

$$\rho_{\sigma\sigma'}(\mathbf{p},\mathbf{p}')=<\hat{a}^{+}_{\mathbf{p},\sigma}\ \hat{a}_{\mathbf{p}',\sigma'}>, \tag{4}$$

where the nondiagonal elements are interband polarization $P_{\mathbf{k}}(t)=<\hat{v}^{+}_{\mathbf{k}}(t)\hat{c}_{\mathbf{k}}(t)>$ and $P^{*}_{\mathbf{k}}(t)=<\hat{c}_{\mathbf{k}}{}^{+}(t)\hat{v}_{\mathbf{k}}(t)>$ ($\hat{v}^{+}_{\mathbf{k}}(t)$ ($\hat{c}_{\mathbf{k}}{}^{+}(t)$) is the creation operator in the valence (conduction) band. Using this formalism and Eqs. (1)-(4) one can obtain the evolution equation for $P_{\mathbf{k}}(t)$ (for different values of k_x, k_y) in the presence of Coulomb interaction and in the linear regime of external laser field:

$$i\hbar\,\partial P_{\mathbf{k}}(t)/\partial t=\Sigma(\mathbf{k})P_{\mathbf{k}}(t)+\Lambda(\mathbf{k}), \tag{5}$$

where for renormalized energy $\Sigma(\mathbf{k})$ and for renormalized Rabi frequency $\Lambda(\mathbf{k})/\hbar$ we obtain the analytical expressions (see Ref [9]).

$$\Sigma(\mathbf{k}) = 2\varepsilon_{\mathbf{k}1} + \sum_{\mathbf{q}\neq 0} V_{2D}(q) T(\varepsilon_{\mathbf{k}}, U, P_{\mathbf{k}}(t)) \tag{6}$$
$$\Lambda(\mathbf{k}) = \mathbf{E}(t)\mathbf{d}(\mathbf{k}) + \sum_{\mathbf{q}\neq 0} V_{2D}(q) \mathrm{P}(\varepsilon_{\mathbf{k}}, U, P_{\mathbf{k}}(t)).$$

Here $V_{2D}(q)$ is the Fourier transform of two-dimensional Coulomb interaction, and electric field of laser pulse has the following form: $E(t) = \exp(-i\omega t)\exp[-(t/\tau)^2]$, with $\tau >> 2\pi/\omega = T$. We solve obtained integral-differential equations numerically in order to obtain the interband polarization $P_{\mathbf{k}}(t)$ and define the macroscopic polarization: $P(t) = \sum_{\mathbf{k}} P_{\mathbf{k}}(t) d^*(\mathbf{k}) + c.c.$

Using Fourier transform of macroscopic interband polarization, we compute the optical susceptibility, and get the excitonic absorption coefficient as complex part of the optical susceptibility.

2.2. Variational approach for impurity states in gapped bilayer graphene

Since there is no analytical solution for the Coulomb problem in bilayer graphene with opened energy gap, in this section we develop a variational approach. The equation for determination of hydrogen-like impurity energy spectrum in gapped graphene bilayer can be presented in the form

$$H_0 \begin{pmatrix} \phi \\ \chi \end{pmatrix} = \left(E + \frac{Ze^2}{r} \right)^2 \begin{pmatrix} \phi \\ \chi \end{pmatrix}, \tag{7}$$

with H_0 given by Eq.(1). From the system of two equations (Eq.(7)) we can obtain one equation for the spinor component ϕ:

$$\left[\frac{U^2}{4} + (v_3 \hat{p})^2 - \frac{v_3 \hat{p}^3}{m} \cos 3\theta + (\frac{\hat{p}^2}{2m})^2 \right] \phi = \left(E + \frac{Ze^2}{r} \right)^2 \phi. \tag{8}$$

For the ground state energy of an impurity electron we choose the variational function in cylindrical coordinates as

$$\phi = N \exp(-\lambda \rho^2), \tag{9}$$

where λ is variational parameter and N is the normalization constant $N = (2\pi \int_0^\infty e^{-2\lambda\rho^2} \rho d\rho)^{-1/2}$.

As a first step, we do not take into account the azimuthal asymmetry of the bands, therefor, in Eq. (8) we ignore the term ($-v_3\hat{p}^3\cos 3\theta/m$) that is responsible for the trigonal warping of the bands [4, 7].

Using dimensionless units for the energy and length: $\tilde{E}=E/R$, $\tilde{U}=U/R$, $\tilde{\rho}=\rho/a_B$ with $R=\mu e^4/2\chi^2\hbar^2$ being the effective Rydberg energy, χ is the dielectric constant and $a_B=\hbar^2\chi/\mu e^2$ is the effective Bohr radius, Eq.(8) leads to the form

$$\left(\tilde{E}^2+\frac{4\tilde{E}}{\rho}+\frac{4}{\rho^2}-\tilde{U}^2\right)\phi=\hat{\mathbf{p}}^2\left(\frac{4}{\alpha^2}+\left(\frac{\mu}{m}\right)^2\hat{\mathbf{p}}^2\right)\phi, \tag{10}$$

where $\alpha=e^2\chi^2/\hbar^2v_3^2$ is the effective fine structure constant that corresponds to the velocity v_3; the mass m in Eq.(8) is defined by the expression $m=\gamma_1/2v_F^2\approx 0.03m_0$ [3] and for effective Rydberg we use the value of $\mu=0.02m_0$ where m_0 is the free electron mass. The operator $\hat{\mathbf{p}}^4$ in Eq. (10) can be considered as double action of the operator $\hat{\mathbf{p}}^2$ in the consecutive order. The ground state energy of the impurity electron can be obtained from following equation

$$\tilde{E}^2+4\tilde{E}\frac{J_1}{N}-\tilde{U}^2+C=0, \tag{11}$$

where C is:

$$C=\frac{4J_2}{J_0}-\frac{16}{\alpha^2}\left(\lambda-\frac{\lambda^2J_3}{J_0}\right)-16\left(\frac{\mu}{m}\right)^2\left(2\lambda^2-4\lambda^3\frac{J_3}{J_0}+\lambda^4\frac{J_4}{J_0}\right), \tag{12}$$

and the integrals J_i are given by the expressions:

$$J_1=\int_0^\infty e^{-2\lambda\rho^2}d\rho,\ J_2=\int_0^\infty\frac{e^{-2\lambda\rho^2}}{\rho}d\rho,\ J_3=\int_0^\infty e^{-2\lambda\rho^2}\rho^3d\rho,\ J_4=\int_0^\infty e^{-2\lambda\rho^2}\rho^5d\rho.$$

3. Results and Discussions

In Fig.1 we present our results obtained for excitonic absorption of gated graphene bilayer as a function of the detuning parameter $\beta=(\hbar\omega-U)/R^*$ for different values of opened energy gap U.

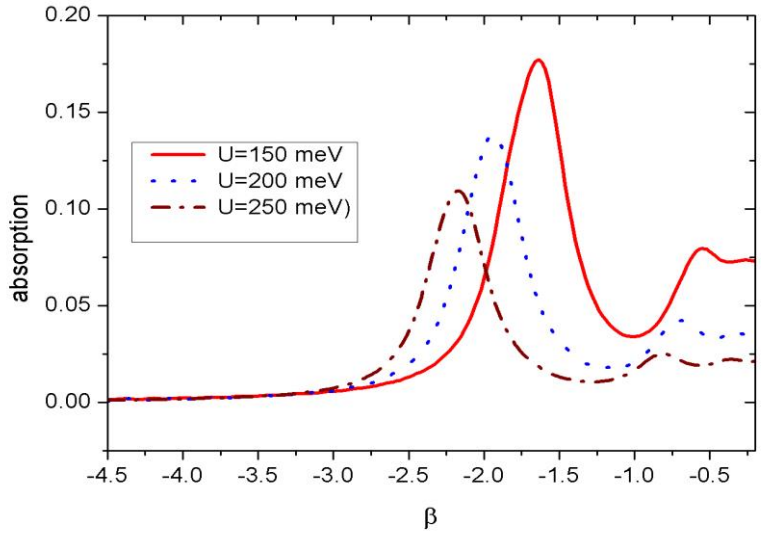

Figure 1. Excitonic absorption in bilayer graphene as a function of the detuning $\beta=(\hbar\omega-U)/R^*$ for different values of the gap: red (solid) line is for U=150 meV; blue (dotted) line corresponds to U=200 meV, and brown (dash-dotted) line is for U=250 meV.

In numerical calculations we introduced dumping constant equal to 0.2 effective Rydberg. We found that intensity of the excitonic absorption increases with decreasing of the gap.

The position of the maximum of absorption curve corresponds to the exciton binding energy: the corresponding value of the photon energy $\hbar\omega_0$ determines the excitonic level position in the gap, while the value $U-\hbar\omega_0$ is the distance of this level from the conduction band bottom and is the exciton binding energy E_B (E_B=1.94 R with $R=2\,meV$ for $U=200\,meV$). As we see in Fig.1, the binding energy increases with the increase of the gap value.

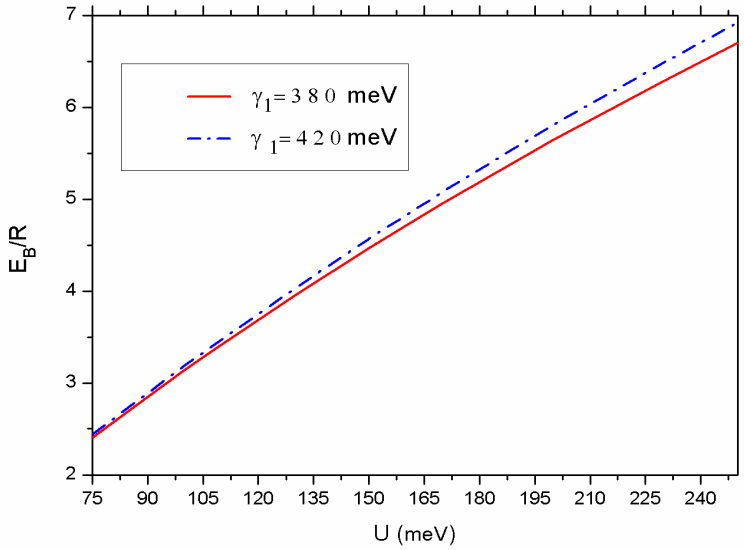

Figure 2. Dependence of the binding energy of impurity electron in effective Rydberg ($R=2\,meV$) on the gap value U at different values of γ_1

Fig.2 shows our results for the dependence of impurity electron binding energy on the value of the opened energy gap U in bilayer graphene obtained on the base of minimization procedure for the energy obtained from Eq. (11). We observe a monotonic increase of the impurity electron binding energy (in the region of about ten *meV*) with the increase of the gap energy. Such behaviour is in the accordance with the tendency obtained for the excitonic case.

4. Conclusions

Thus, in this paper we study the dependence of excitonic and impurity states on the value of the gap introduced by a static electric field. For excitonic states we used tight-binding approach with second quantized Hamiltonian, while for impurity states we develop a variational approach. In both cases we obtained similar behaviour for binding energy: we observe a monotonic increase of binding energy with the increase of the gap. We found that the binding energy of an impurity electron in bilayer graphene is about ten *meV* and can be tuned by electric field.

References

[1] A.V. Andrianov, A.O. Zakhar'in, Yu.L. Ivanov, and M.S. Kipa, JETP Letters 91, 96 (2010)
[2] K. Geim and K.S. Novoselov, Nature Materials 6, 183 (2007)
[3] E. McCann and V.I. Fal'ko, PRL 96, 086805 (2006)
[4] E. McCann, Phys. Rev. B 74, 161403 (2006)
[5] E.V. Castro, K. S. Novoselov et al., Phys. Rev. Lett. 99, 216802 (2007)
[6] W. Bao, et al, Nature Physics 7, 948 (2011)
[7] A.A. Avetisyan, B. Partoens, and F.M. Peeters, Phys. Rev. B 81, 115432 (2010)
[8] A.A. Avetisyan, B. Partoens, and F.M. Peeters, Phys. Rev. B 80, 195401 (2009)
[9] A.A. Avetisyan, A. Djotyan, and K. Moulopoulos, Physics of Atomic Nuclei, 80, No. 2, 307 (2017)
[10] I.S. Makhov et al., St. Petersburg Polytechnical University Journal: Physics and Mathematics, 2, 281 (2016)
[11] J. Nilson and A.H. Castro Neto, arXiv:cond-mat/0612470v2
[12] N.M.R. Peres, R.M. Ribeiro, and A.H. Castro Neto, Phys. Rev. Lett. 105, 055501 (2010)
[13] V.M. Kuleshov et.al., JETP Letters, 101, 282-288 (2015)