UDC 661.666-022.532.01(043)

A STRONG ELECTROMAGNETIC RADIATION INTERACTION WITH BILAYER GRAPHENE

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We develop a microscopic theory of a strong electromagnetic radiation interaction with bilayer graphene where an energy gap can be opened by using external gates that create a static electric field perpendicular to graphene planes. We show that an adiabatic change on time of the gate potentials (that leads to the resonance of the energy gap with an electromagnetic field) may produce full inversion of the electron population between valence and conduction bands. Quantum kinetic equations for density matrix are obtained by the use of a tight-binding approach within the second quantized Hamiltonian in an intense laser field.

Keywords: bilayer graphene, intensive electromagnetic radiation, inversion of population.

Introduction. Since the experimental discovery of graphene [1], that is a two-dimensional (2D) crystal of carbon atoms packed in hexagonal lattice [1, 2], it has become an important research area in material science and condensed-matter physics. This activity is stimulated by the successful fabrication of stable ultrathin graphite films with excellent mechanical quality, exotic energetic spectrum which are very promissing for e.g. nanoelectronics [3] and as transparent conducting layers [4].
Graphene has been extensively considered as a promising material for nonlinear optical applications [5, 6]. A theoretical investigation of nonlinear electromagnetic properties of monolayer graphene, for the case when multiphoton interband excitation is induced by a laser radiation is studied in Ref. [6].

Theoretical and experimental investigations on the nonlinear effects induced in graphene system so far have been mainly focused in monolayer graphene. Meanwhile, in the physics of graphene there is growing interest in bilayer and trilayer graphene systems, where the electronic band structures are richer than in monolayer graphene [7, 8]. It is interesting to investigate these effects in multilayer graphene systems.

A desirable band structure for multilayer graphene systems that can be useful for different purposes of nano- and optoelectronics, can be theoretically found (and proposed for an experimental realization) e.g. by the corresponding choice of the layer number in a graphene system.

Alternatively, the band structure can be tuned by the application of external fields. 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, which is tunable by the gate voltage [9]. Magnetotransport [10] showed that the induced gap between the conduction and valence bands could be tuned between zero and midinfrared energies.

In [11, 12] we studied theoretically electric field induced band gaps of graphene multilayers with different ways of stacking between consecutive graphene planes. Using a positively charged top and a negatively charged back gate, it is possible to control independently the density of electrons on the graphene layers (correspondingly the band gap) and the Fermi energy of multilayer graphene systems.

Optical measurement techniques are widely adopted to experimentally investigate electronic properties of multilayers of graphene. To determine the number of layers as well as the stacking structure Raman spectroscopy was used in Refs [13, 14]. Infrared spectroscopy is also applied to probe the low-energy band structure. The dependence of the infrared optical absorption on the stacking sequence has been observed in recent experiments [15].

In the present paper, the microscopic theory of a strong electromagnetic radiation interaction with bilayer graphene with opened band gap is developed. We consider one-resonant interactions of a laser field with bilayer graphene, with coherent superposition states induced by the laser radiation. Our analysis is based on a tight-binding approach of the second quantized Hamiltonian in an intense laser field.

Theory. Here, we consider the interaction of a strong electromagnetic wave with bilayer graphene. A perpendicular electric field created by top and back gates [11, 12] opens an energy gap in multilayer graphene. We assume that the laser pulse propagates in the perpendicular direction to graphene plane (XY) and the electric field $\boldsymbol{E}(t)$ of pulse lies in the graphene plane, which allows to exclude the effect of the wave magnetic field.

The Hamiltonian in the second quantization formalism has the form:

$$H = \int \Psi^{+} H_s \Psi d\mathbf{r} \,. \tag{1}$$

The Hamiltonian H for bilayer in the vicinity of the K point can be written as (here we omit the real spin and valley quantum numbers):

$$H_s = H_0 + H_d \,, \tag{2}$$

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

$$H_d = \begin{pmatrix} e\mathbf{r}\mathbf{E}(t) & 0 \\ 0 & e\mathbf{r}\mathbf{E}(t) \end{pmatrix}.$$

The first term in Eq. (2) corresponds to bilayer graphene in the field of perpendicular electric field, and the second term is the interaction Hamiltonian between a laser field and bilayer graphene, with $v_3 \approx v_F/8$ is the effective velocity (v_F is the Fermi velocity in monolayer graphene), U is the gap introduced by the perpendicular electrical field, $\mathbf{p}=\{p_x,p_y\}$ is the electron momentum operator. We expand the fermionic field operator over the free wave function $\psi_{p\sigma}(\mathbf{r},t)$ of bilayer graphene:

$$\Psi(r,t)=\sum_{p\sigma}\hat{a}_{p,\sigma}(t)\psi_{p,\sigma}(r,t)\ , \tag{3}$$

where the annihilation operator $\hat{a}_{p,\sigma}(t)$ is associated with positive and negative energy solutions $\sigma=\pm 1$. Introducing $\theta(p)=\arctan(p_y/p_x),\ p_x+ip_y=p\exp(i\theta)$ the expression for energy spectrum of bilayer graphene can be presented in the form:

$$\varepsilon_{p,\sigma}=\sigma\sqrt{\frac{U^2}{4}+(v_3p)^2-\frac{v_3p^3}{m}\cos 3\theta+(\frac{p^2}{2m})^2}\ . \tag{4}$$

The free solutions in bilayer graphene $\psi(\mathbf{r},t)$ have the following form:

$$\psi(r,t)=e^{\frac{i}{\hbar}\mathbf{pr}}\psi_{\sigma}(\mathbf{p})=\frac{\sqrt{\varepsilon_{p\sigma}+U/2}}{\sqrt{2\varepsilon_{p\sigma}}}\begin{pmatrix}1\\ \dfrac{1}{\varepsilon_{p\sigma}+U/2}\gamma(p,\theta)\end{pmatrix}, \tag{5}$$

where

$$\gamma(p,\theta)=-\frac{p^2}{2m}\exp(i2\theta)+v_3p\exp(-i\theta).$$

Laser interaction with bilayer graphene system in an external electric field. Taking into account Eqs. (1)-(3) the second quantized Hamiltonian for the single-particle part can be expressed in the form:

$$\hat{H}=\sum_{\mathbf{p},\sigma}\varepsilon_{\sigma}(p)\hat{a}^{+}_{\mathbf{p},\sigma}\hat{a}_{\mathbf{p},\sigma}+e\mathbf{E}(t)\sum_{\mathbf{p},\sigma}\sum_{\mathbf{p}',\sigma'}\mathbf{D}_{\sigma\sigma'}(\mathbf{p},\mathbf{p}')\hat{a}^{+}_{\mathbf{p},\sigma}\hat{a}_{\mathbf{p}',\sigma'}\ . \tag{6}$$

For the dipole matrix element

$$\mathbf{d}_{\sigma\sigma'}(\mathbf{p},\mathbf{p}')=ie\mathbf{D}_{\sigma\sigma'}(\mathbf{p},\mathbf{p}')\,, \tag{7}$$

where

$$\mathbf{D}_{\sigma\sigma'}(\mathbf{p},\mathbf{p}') = \psi^{+}{}_{\sigma}(\mathbf{p})\,\psi_{\sigma}(\mathbf{p}')\frac{1}{\mathrm{S}}\int \mathbf{r}\, e^{\frac{i}{\hbar}(\mathbf{p}'-\mathbf{p})} d\,\mathbf{r}\,, \tag{8}$$

we obtained an expression, which we do not bring here due to its long form. In contrast to the non-relativistic case, we have found that the dipole matrix element for the light interaction with the bilayer depends on electron momentum.

We use the Heisenberg representation, where the operator evolution is given by the following equation

$$i\hbar\frac{\partial \hat{L}}{\partial t} = [\hat{L}, \hat{H}]\,. \tag{9}$$

The single-particle density matrix in the momentum space is defined as:

$$\rho_{\sigma\sigma'}(\mathbf{p},\mathbf{p}') = < \hat{a}^{+}_{\mathbf{p},\sigma}\ \hat{a}_{\mathbf{p}',\sigma'} > . \tag{10}$$

Using Eqs. (6)-9) one can obtain the evolution equation for the single-particle density matrix for different $\mathbf{p}$ values, and in the presence of an external laser field:

$$\partial\rho_{1-1'}(\mathbf{p},\mathbf{p},t)/\partial t = \frac{2\varepsilon_1(p)}{i\hbar}\rho_{1-1}(\mathbf{p},\mathbf{p},t) + \frac{E(t)d(t)}{\hbar}[\rho_{11}(\mathbf{p},\mathbf{p},t) - \rho_{-1-1}(\mathbf{p},\mathbf{p},t)], \tag{11}$$

$$\partial\rho_{11}(\mathbf{p},\mathbf{p},t)/\partial t = \frac{E(t)d(t)}{\hbar}[\rho_{1-1}(\mathbf{p},\mathbf{p},t)\,d^{*}(\mathbf{p}) + d(\mathbf{p})\rho_{-11}(\mathbf{p},\mathbf{p},t)]\,,$$

where the index $\sigma = 1$ is connected with the conduction band and the index $\sigma = -1$ is related to the valence band..

Discussion. In the present paper, the microscopic theory of a strong electromagnetic radiation interaction with multilayer graphene systems is developed. We consider one-resonant interaction of a laser field with bilayer graphene when an energy gap U is opened due to external gates. It has been found that by changing the energy gap linearly on time, the electron population is transferred from the top of valence band to the bottom of conduction one after the time t_{f}, when the gap comes into resonance with the electromagnetic field. This is an alternative and a more suitable way to bring the system into the resonance in comparison with the method of frequency chirped pulse. The obtained 2D plot for the evolution of particle distribution function $\rho_{cc}(\mathbf{p},\mathbf{p}) = < \hat{a}^{+}_{\mathbf{p},\sigma}\ \hat{a}_{\mathbf{p},\sigma} > = N_c$ (in the conduction band) as a function of time is shown in Fig. 1 for the pulse having $\hbar\omega_0 = 32E_L$ with ω_0 its frequency (in units of the Lifshitz energy $E_L = mv_L^2/2 = 1meV$ and the momentum

$p_L = mv_L$). For this case, during the interaction time t_f =100T, the energy gap of bilayer graphene reaches its maximal final value $U_{fin} = 28E_L$. For this case, i.e. for $\hbar\omega_0 > U_{fin}$, the electrons transfer to the conduction band in the region which is higher than the conduction band bottom (see the band structure for multilayers of graphene in Ref. [12]) where we found that the bottom of the bands as well as the higher isoenergetic levels have trigonal shape) into the isoenergetic line. As shows Fig., at the beginning of the interaction, the population of electrons in the conduction band is negligible (that corresponds to light contour in Fig.) while at the end of the interaction we observe full inversion of the population of electrons between the valence and the conduction bands. (that corresponds to dark contour in Fig.) .

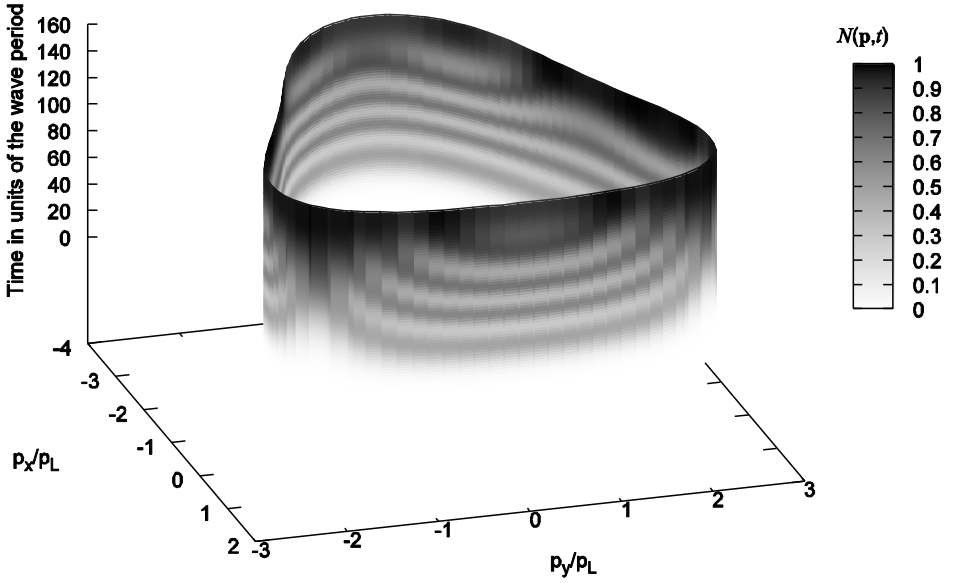

Fig. The evolution of the particle distribution function Nc(p) (in arbitrary units) during the interaction with the pulse with $\hbar\omega_0 = 32E_L$, and the energy gap of bilayer graphene reaches its maximal final value $U_{fin} = 28E_L$ (dark color corresponds to the maximum of the population, i.e. Nc(p)=1)

Conclusion. Since the values of the induced gap in graphene systems are in *THz* region, and producing of a frequency chirp for far infrared laser (terahertz laser) is

difficult at present and highly inefficient, here we consider an alternative way to produce the inverse population.

The essence of the proposed method is to use the graphene system where the energy gap is a linearly increasing function of time. This can be achieved by adiabatically changing the potential on the gates.

Such a scheme can be more convenient from experimental point of view and useful for "on demand" creation of coherent superposition of quantum states, and for creating new optoelectronic devices.

***Acknowledgements*.** The author thanks Dr. G.F. Mkrtchian and Prof. V.V. Buniatyan for fruitful discussions.

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Received on 22.09.2014.
Accepted for publication on 17.12.2014.

ԻՆՏԵՆՍԻՎ ԼԱԶԵՐԱՅԻՆ ԴԱՇՏԻ ԵՎ ԵՐԿՇԵՐՏ ԳՐԱՖԵՆԻ ՓՈԽԱԶԴԵՑՈՒԹՅՈՒՆԸ

Ա.Ա. Ավետիսյան

Զարգացվել է միկրոսկոպիկ տեսություն՝ ինտենսիվ լազերային դաշտի և երկշերտ գրաֆենի համակարգի փոխազդեցությունը նկարագրելու համար, երբ համակարգում առկա է էներգիական ճեղք՝ ստեղծված հաստատուն էլեկտրական դաշտով: Լազերային ճարագայթման և համակարգի միջև մեկ ֆոտոնային ռեզոնանսային փոխազդեցության շրջանակներում ուսումնասիրվել են դաշտով ստեղծված կոհերենտ վիճակները երկշերտ գրաֆենում: Ցույց է տրվել, որ ժամանակի ընթացքում էլեկտրական դաշտ ստեղծող

փականի պոտենցիալի ադիաբատիկ փոփոխությունը (որը հանգեցնում է ռեզոնանսի էլեկտրամագնիսական դաշտի և էներգիական ճեղքի միջև) կարող է առաջացնել էլեկտրոնային բնակեցվածության լրիվ ինվերսիայի արժեքական և հաղորդականության գոտիների միջև: Խտության մատրիցի համար, երկրորդական քվանտացման մեթոդի հիման վրա ստացվել են քվանտային կինետիկ հավասարումներ՝ երկշերտ գրաֆենի համակարգին կիրառված ինտենսիվ լազերային դաշտի պայմաններում:

Առանցքային բառեր. երկշերտ գրաֆեն, ինտենսիվ լազերային դաշտ, բնակեցվածության ինվերսիա:

ВЗАИМОДЕЙСТВИЕ ИНТЕНСИВНОГО ЛАЗЕРНОГО ИЗЛУЧЕНИЯ С ДВУХСЛОЙНЫМ ГРАФЕНОМ

А.А. Аветисян

Развита микроскопическая теория для описания взаимодействия интенсивного лазерного излучения с двухслойным графеном при наличии энергетической щели, созданной электрическим полем, перпендикулярным к слоям графена. Рассмотрено однофотонное резонансное взаимодействие между лазерным излучением и двухслойным графеном и исследованы созданные лазерным полем когерентные состояния. Показано, что адиабатическое изменение во времени потенциала на затворе, создающего электрическое поле (в условиях резонанса между электромагнитным полем и энергетической щелью), может привести к полной инверсии электронной заселенности между валентной зоной и зоной проводимости. Получены квантовые кинетические уравнения для матрицы плотности на основе метода вторичного квантования для случая, когда двухслойная графеновая система находится в поле сильного лазерного излучения.

Ключевые слова: двухслойный графен, интенсивное лазерное излучение, инверсия заселенности.