# Photoinduced State of Floquet Insulator in Graphene-like Crystal

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Floquet spectrum of charge carriers in a 2*D*-crystal with initially displaced Dirac points has been derived. The phase and amplitude dependences of the energy gap induced by elliptically polarized and bichromatic high-frequency fields has been investigated. In contrast to graphene the linearly polarized electric field has been shown to be able to transform the initially semi-metallic state of Dirac crystal into the Floquet-insulator state. The conditions for such a transition are indicated, one of which is the mismatch between the orientation of the field polarization line and the direction of the crystallographic axes.

Keywords: Floquet Spectrum, Quasienergy, Dirac Crystal, Semi-Dirac Crystal, Graphene, Floquet Topological Insulator.

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# Introduction

Electronics development is inextricably connected with creation of new nanomaterials. Modern technologies allow to derive low-dimension structures of various type, including 2D-crystals of monoatomic thickness [1,2]. Discovering such classes of solid-state structures as Dirac and Weyl crystals is of practical [3–5] and fundamental importance. It is well known, that free graphene is characterized with conic type of dispersion law, i.e. linear dependence between energy and pulse of electron. While graphene on a substrate can correspond to hyperbolic type of the dispersion law [6]. Such mathematical similarity of electron states in low-dimensional systems physics and high energy physics allows to use modern nanomaterials as a model of some effects of quantum electrodynamics [7,8].

At present time the study of anisotropic models of Dirac crystals is of interest [9-13]. Thus, for instance, the so called semi-Dirac crystals were made in laboratory conditions [14], where square dispersion corresponds to the charge carriers movement along one crystallographic axis, while linear or hyperbolic dispersion — to movement along another. As an example, such crystals can include phosphorene [15] or graphene, subject to mechanical stress along some direction [16]. Graphene tension results in non-equivalent Dirac points drawing together, that can happen until their merging. In the latter case the Hamiltonian of the system is of semirelativistic nature in the above mentioned meaning [17].

Increasing number of works on studying the effects of dynamic (topological) modification of energy structure of

Dirac and semi-Dirac materials by means of their interaction with laser radiation is explained the following way. First of all, the so called Floquet topological insulators have been already implemented in laboratory conditions [18-20]. Theory of dynamic application of dielectric state of Dirac systems is developed in [21–23]. Particularly, in [22] the solutions of equation, describing the related electronphoton states in graphene, subject to circularly polarized electromagnetic radiation, were observed. Secondly, tasks on crystal interaction with radiation are non-stationary and, as noted in [24], the effects, appearing in such systems, are much remarkable and richer, than in the same systems, but described with stationary Hamiltonian. Among them are the modification of the structure of Landau levels in 2D-electron gas [25,26], manipulation with position of Dirac points [24,27-29], dynamic application of the forbidden band [21-23,30-32], Dirac points merging, induced with high-frequency (HF) field [33], successive transitions between semi-metallic phases and states of insulator [33,34], Fermi velocity renormalization [35], modification of graphene spectra in quantizing magnetic field [35,36], etc.

In [34] under the model of electron spectrum of graphene-like material with displaced Dirac points [17] the expression for dependence of quasi-energy gap on intensity of incident radiation, polarized in circle, was successfully derived. Floquet spectrum [34] allows to analytically describe the alternating transitions between the states of semi-metal and band insulator. The possibility of transition of 2D Dirac semi-metal to the band insulator state in case of arbitrary polarization of HF field is investigated below.

Particularly, it is demonstrated, that at certain conditions the quasi-energy gap can appear (a) for linear polarization and also (b) in case of interaction with bichromatic field, that can not be explained under conic spectrum model [30].

# 1. Graphene-like material in HF field

It is known, that change of values of the nearest atoms overlap integrals (caused, for instance, by mechanical stress) results in Dirac points drawing together in Brillouin zone. Effective Hamiltonian, describing such situation, is observed in [17] and written as

$$\hat{H}(\mathbf{p}) = v_{\rm F} p_x \hat{\sigma}_x \psi + (\alpha p_y^2 - \Delta) \hat{\sigma}_y \psi, \qquad (1)$$

where  $\hat{\sigma}_{x,y,z}$  are Pauli matrices,  $\alpha$  and  $\Delta$  are parameters, defined with overlap integrals. Phase transition from semimetal state into the band insulator state happens when parameter  $\Delta$  changes the sign. Hereinafter, let's assume, that  $\Delta > 0$  and, as a result, there are two Dirac points, located symmetrically on axis  $p_y$  on both sides from point  $\mathbf{p} = 0$ . Distance between them in  $\mathbf{p}$  space is  $2\sqrt{2m\Delta}$ , where  $m = 1/2\alpha$ .

Now let's assume, that 2*D*-crystal, charge carriers of which are described with Hamiltonian (1), interacts with HF electric field, potential of which is equal to

$$\mathbf{A}_{\rm ac} = -\frac{c}{\omega} \big( E_1 \sin(n\omega t + \varphi), E_2 \sin \omega t \big). \tag{2}$$

Here, n = 1 or 2, wherein if n = 1, then  $\varphi$  means phases displacement between oscillations of mutually orthogonal constituents of the electric field intensity.

Under Floquet formalism [37] quantum-mechanical state of electron in graphene-like crystals, interacting with periodic field, is described with two-component spinor u(t), components of which are time-periodic functions with period  $2\pi/\omega$ . Spinor *u* satisfies the equation

$$\left[\hat{H}\left(\mathbf{p}+\frac{e}{c}\,\mathbf{A}_{\mathrm{ac}}\right)-i\hbar\frac{\partial}{\partial t}\right]u=\tilde{\varepsilon}u,\tag{3}$$

where  $\tilde{\varepsilon}(\mathbf{p})$  is quasi-energy, for calculation of which the averaging method is used. Stationary constituent  $u_0$  of the spinor u satisfies the equation, observed by averaging (3) over the field period:

$$\hat{H}(\mathbf{p})u_{0} + \frac{p_{2}^{2}}{4m}\hat{\sigma}_{y}u_{0} - p_{1}\upsilon_{F}\left\langle\sin(n\omega t + \varphi)\hat{\sigma}_{x}u_{ac}\right\rangle$$
$$- \frac{p_{2}p_{y}}{m}\left\langle\sin\omega t\hat{\sigma}_{y}u_{ac}\right\rangle - \frac{p_{2}^{2}}{4m}\left\langle\cos 2\omega t\hat{\sigma}_{y}u_{ac}\right\rangle = \tilde{\varepsilon}u_{0}. \quad (4)$$

Here,  $p_{1,2} = eE_{1,2}/\omega$ ,  $u_{ac}(t)$  is spinor HF constituent u,  $\langle u_{ac} \rangle = 0$ . Let's substitute  $u = u_0 + u_{ac}$  to equation (3), leaving only HF components and neglecting the summands, containing  $u_{ac}$ . The latter is justified in case of significantly

high field frequency:  $\hbar \omega \gg \Delta$ ,  $v_F \sqrt{m\Delta}$  [34]. As a results the expression for  $u_{ac}$  takes the form

$$u_{\rm ac} = -\frac{\iota p_1 \upsilon_{\rm F}}{n\hbar\omega} \cos(n\omega t + \varphi)\hat{\sigma}_x u_0 - \frac{\iota p_2 p_y}{m\hbar\omega} \cos\omega t\hat{\sigma}_y u_0 + \frac{i p_2^2}{8m\hbar\omega} \sin 2\omega t\hat{\sigma}_y u_0.$$
(5)

Let's further examine the cases, when n = 1 and 2, since exactly in these cases the summands, averaged in (4), differ from zero.

# 2. Elliptical and linear polarization of HF field

Elliptical polarization corresponds to situation, when n = 1. As a result of averaging in (4) we come down to the next stationary eigenvalue problem:

$$\hat{H}(\mathbf{p})u_0 + \frac{p_2^2}{4m}\hat{\sigma}_y u_0 - \frac{p_1 p_2 p_y v_F \sin \varphi}{m\hbar\omega}\hat{\sigma}_z u_0 = \tilde{\varepsilon} u_0.$$
(6)

The case of circular polarization  $E_1 = E_2$ ,  $\varphi = \pm \pi/2$ is examined in [34], where the possibility of successive transitions between dynamically applied states of semimetal and band insulator is shown. In situation, when  $0 < \varphi < \pi/2$ , this feature remains. However, this effect is the most remarkable exactly for circular polarization. Indeed, for arbitrary phases  $\varphi$  the value of energy gap  $\Delta_g$ in Floquet spectrum  $\tilde{\epsilon}(\mathbf{p})$  is calculated as per the formula

$$\begin{split} \Delta_g &= 2\Delta \\ &\times \begin{cases} 4\sqrt{2}Wb |\sin \varphi| \sqrt{1 - W - 8b^2 W^2 \sin^2 \varphi}, & W < W_A, \\ W - 1, & W > W_A, \end{cases} \end{split}$$

where  $W = p_1^2/4m\Delta$ ,  $b = \sqrt{\mu}/\nu$ ,  $\mu = m\nu_F^2/\Delta$ ,  $\nu = \hbar\omega/\Delta$ ,

$$W_A = rac{-1 + \sqrt{1 + 64b^2 \sin^2 \varphi}}{32b^2 \sin^2 \varphi}.$$

As seen, at  $W < W_A$  the value of  $\Delta_g \to 0$  at  $\varphi \to 0$  or  $\varphi \to \pm \pi$ . However, in case of linear polarization the system maintains the possibility of dynamic transition to the band insulator state. This could be verified by putting  $\varphi = 0$  and  $p_2 = p_0 \sin \theta$  into (6):

$$\hat{H}(\mathbf{p})u_0 + \frac{p_0^2 \sin^2 \theta}{4m} \,\hat{\sigma}_y u_0 = \tilde{\varepsilon} u_0. \tag{8}$$

Here,  $p_0 = \sqrt{p_1^2 + p_2^2}$ ,  $\theta$  is angle between polarization line and axis Ox. Using (8) we get the quasi-energy

$$\tilde{\varepsilon} = \pm \Delta \sqrt{q_x^2 + (q_y^2 - 1 + W_0 \sin^2 \theta)^2},\tag{9}$$

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**Figure 1.** Structure of Floquet spectrum in case of bichromatic HF field; a — constant quasi-energy lines (in  $\Delta$  units) at W = 0.5; b-d — dependence of quasi-energy on dimensionless quasi-pulse  $q_y$ ; b - W = 0.5; c — annihilation of maximums of quasi-energy at W = 1.0; d - W = 1.2.

where  $q_x = v_F p_x / \Delta$ ,  $q_y = p_y / \sqrt{2m\Delta}$ ,  $W_0 = p_0^2 / 4m\Delta$ . As a result, we get the following expression for the quasi-energy gap:

$$\Delta_g = 2\Delta (W_0 \sin^2 \theta - 1) \Theta (W_0 \sin^2 \theta - 1).$$
(10)

Here,  $\Theta(\xi)$  is a step function. As per (10), the following conditions should be met for dynamic transition to the band insulator state in case of linear polarization. First of all, the HF field polarization line should constitute nonzero angle with axis Ox, i.e. the electric field intensity vector should always has nonzero constituent for axis, movement along which is described with quadratic spectrum. Secondly, transition to the insulator state happens only after annihilation of Dirac points, i.e. at

$$W_0 > 1 + \operatorname{ctg}^2 \theta. \tag{11}$$

It should be noted, that annihilation happens at relatively high radiative power. Considering the numerical values of the spectrum parameters [16], the dimensionless parameter  $W_0 = 1$  ( $\theta = \pi/2$ ) is corresponded to the intensity  $I = 500 \text{ mW}/\mu\text{m}^2$ . Let's evaluate the value of quasienergy gap, induced with linearly polarized radiation with intensity  $I = 510 \text{ mW}/\mu\text{m}^2$  (W = 1.02 > 1). As per (10), it is  $\Delta_g = 2 \text{ meV}$ . Quasi-energy gap, calculated under conic model and applied with the circularly polarized field of the same power, will be, as per [30],  $\Delta_0 = 0.1 \text{ eV}$ . Thus,  $\Delta_g/\Delta_0 \sim 0.02$ . The possibility of the described transition is caused by consideration of the end distance between the Dirac points in quasi-pulses space. Indeed, when transitioning into the coordinate system of **p** space, where one of the Dirac points of model (1) is taken as the origin of coordinates, then the coordinate of the second Dirac point on axis  $p_y$  will be  $2\sqrt{2m\Delta}$ . Thus, the model Hamiltonian (1), based on which the result (10) is observed, degenerates into the conic model, if  $\sqrt{m\Delta} \gg p_0$ . Here, *m* and  $\Delta$  are expressed through parameters of a lattice and overlap integrals [17]. As was stated earlier, one of the required conditions for quasi-energy gap opening is a dynamic annihilation of Dirac points. The latter is implemented at satisfying the inequation (11), that is equivalent to

$$p_0^2 > 4m\Delta(1 + \operatorname{ctg}^2 \theta) > m\Delta.$$
<sup>(12)</sup>

Inequation can not be implemented under conic model, valid at  $\sqrt{m\Delta} \gg p_0$  (technically the parameter  $(m\Delta)^{-1} = 0$  leads to the fact that the step function in formula (10) will always yield zero).

# 3. Bichromatic HF field

As was stated above, the nonzero averaged summands in (4) are also possible, if HF radiation, with which 2Dcrystal interacts, is bichromatic. Indeed, if we put n = 2



**Figure 2.** Dependence of quasi-energy gap on dimensionless intensity of HF field for  $\hbar \omega = 10\Delta$  (line *I*),  $\hbar \omega = 20\Delta$  (line *2*),  $\hbar \omega = 50\Delta$  (line *3*). Point A corresponds to annihilation of minimums of the Floquet spectrum.

into (4) and (5), then after averaging we will get the following stationary task:

$$\hat{H}(\mathbf{p})u_0 + \frac{p_2^2}{4m}\hat{\sigma}_y u_0 + \frac{p_1 p_2^2 v_F \cos\varphi}{8m\hbar\omega}\hat{\sigma}_z u_0 = \tilde{\varepsilon}u_0.$$
(13)

It should be noted, that here  $p_1, p_2 \neq 0$ , since otherwise we will deal with monochromatic field again and with linear polarization. Without loss of generality let's assume that  $p_1 = p_2$ . Then the Floquet spectrum of charge carriers will be

$$\tilde{\varepsilon} = \pm \Delta \sqrt{q_x^2 + (q_y^2 - 1 + W)^2 + b^2 W^3 \cos^2 \varphi}.$$
 (14)

Structure of the Floquet spectrum (14) is graphically presented in Fig. 1. With HF field appearing the Dirac points disappear. Instead of them the quasi-energy minimums appear (points M in Fig. 1, a, b) and quasi-energy gap appears, equal to

$$\Delta_{g} = 2\Delta \begin{cases} bW^{3/2} |\cos \varphi|, & W < 1, \\ \sqrt{(W-1)^{2} + b^{2}W^{3}\cos^{2}\varphi}, & W > 1. \end{cases}$$
(15)

With increase of radiation intensity the minimums come close to each other and at W = 1 their annihilation is performed (point A in Fig. 1, c), similar to dynamic annihilation of Dirac points in [33]. But in contrast with [33,34] the further increase of the field amplitude does not result in collapse of the forbidden band and appearing of the new Dirac point. At W > 1 quasi-energy gap continues to increase, while the Floquet spectrum takes the semi-Dirac form: at low pulses ( $|q_y| \ll 1$ ) the movement along axis Oy is described with quasi-energy, quadratic over the pulse  $p_y$  (Fig. 1, d). Effective mass, renormalized with HF field action, in this case is equal to

$$m_{\rm eff} = \frac{m}{W-1} \sqrt{(W-1)^2 + b^2 W^3 \cos^2 \varphi}, \ W > 1.$$
(16)

Dependence of quasi-energy gap on dimensionless intensity of the field, built as per formula (15) for various values of parameter  $v = \hbar \omega / \Delta$ , is shown in Fig. 2, where point A corresponds to the moment of annihilation of the Floquet spectrum minimums. Let's compare the value of quasienergy gap (15), applied in 2*D*-crystal with bichromatic field at  $\varphi = 0$ , with the value of the gap  $\Delta_0$ , induced with circularly polarized HF field [30]. As per [30], if  $I = 130 \text{ mW}/\mu\text{m}^2$  and  $\hbar \omega = 140 \text{ meV}$ , then  $\Delta_0 = 27 \text{ meV}$ . At the same intensity and frequency the value of the gap from the bichromatic field, as per formula (15), is equal to  $\Delta_g = 2.5 \text{ meV}$ , that is by an order less than value of  $\Delta_0$ .

# Conclusion

Analysis of results of the Floquet spectrum calculation for graphene-like crystal, described with anisotropic Hamiltonian (1), has showed the possibility of the quasi-energy gap appearing even in case of interaction with linearly polarized radiation. However, for that the following conditions should be met. First of all, there should be the nonzero constituent of HF field intensity vector relating to the axis, along which the electrons have quadratic spectrum. Secondly, by means of the field intensity increase the dynamic annihilation of Dirac points should be reached, for the Floquet spectrum of the system to have a semi-Dirac form. It should be noted here, that under conic spectra model, applied for description of the electromagnetic response of graphene [24], the transition to the band insulator state in case of linear polarization of HF field is impossible.

Transition to the band insulator state in case of bichromatic field is caused, first of all, by nonadditivity of the system spectrum (monochromatic constituents are polarized in orthogonal directions). Secondly, presence of the summand, quadratic over the pulse, in Hamiltonian of the system results in doubling of the system response frequency by the field constituent, oscillating along axis Oy with frequency  $\omega$ , and, as a result, to nonzero averaged in (4) summand, providing the examined effect.

#### **Conflict of interest**

The authors declare that they have no conflict of interest.

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