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Generation of multi-mode velocity of electrons in a Dirac crystal in the monochromatic field

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Abstract. Multi-mode dynamics with Zitterbewegung of an electron in 2D Dirac crystal placed in the field of monochromatic radiation is studied. For calculations, a model Hamiltonian taking into account two independent Dirac points has been used. Calculations have shown that the spectrum of electron oscillations contains a series of new (compared to the usual Zitterbewegung) frequencies. The latter, in the case of a high radiation frequency, are a combination of the Zitterbewegung frequency and frequencies that are multiples of the field frequency. In the case when the field frequency is comparable to the Zitterbewegung frequency, the spectrum of electron oscillations is determined by the field amplitude. The character of this dependence has been shown to be changed by variation of the direction of radiation polarization. The possibility of the appearance of a constant component of the electron velocity in the field of monochromatic radiation is also discussed.

Keywords: Zitterbewegung, graphene, Dirac crystal, Rabi frequency

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Генерация многомодовой скорости электронов в дираковском кристалле в монохроматическом поле

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Аннотация. Исследована многомодовая динамика электрона с учетом Zitterbewegung'а в двумерном дираковском кристалле, помещенном в поле монохроматического излучения. Для расчетов использовался модельный гамильтониан, учитывающий две независимые точки Дирака. Расчеты показали, что спектр колебаний электрона содержит ряд новых (по сравнению с обычным Zitterbewegung'ом) частот. Последние, в случае высокой частоты излучения, представляют собой комбинацию частоты Zitterbewegung'а и частот, кратных частоте поля. В случае, когда частота поля сравнима с частотой Zitterbewegung'а, спектр колебаний электрона определяется амплитудой поля. Показано, что характер этой зависимости меняется при изменении направления поляризации излучения. Обсуждается также возможность появления постоянной составляющей скорости электрона в поле монохроматического излучения.

Ключевые слова: Дрожащее движение, графен, дираковский кристалл, частота Раби

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Introduction

The discovery of new types of 2D crystals constituting the group of so-called Dirac materials (graphene, germanene, silicene, etc.), as well as the study of their electrodynamics properties, determined essentially the development of that part of the physics of solid-state structures that stands at the junction of the condensed matter theory and high energy physics. The point is that the relativistic form of the equations for electron states in 2D hexagonal lattices makes graphene-like materials a convenient platform to study the effects of quantum electrodynamics [1, 2]. The uniqueness of the above materials is explained by the presence of the components relating the momentum of the charge carrier to its pseudospin degree of freedom in the quantum equation. Examples of manifestation of such a relation are topological phase transitions [3–5], transitions of “semi-metal–band insulator” [4, 6, 7] and “Dirac–semi-Dirac material” [8,9] types, as well as the Zitterbewegung (ZB) – fast oscillations of the velocity of free (pseudo)relativistic electron due to the interference of the states with positive and negative energies.

Previously the possibility of electron ZB had been shown theoretically for Dirac crystals [10, 11], for solid state with Rashba/Dresselhaus spin-orbit coupling and the Zeeman splitting [12], and for strained III-V semiconductors [13,14] as well. However for vacuum the experimental realization of ZB is very difficult due to the high frequency (HF) of the corresponding electron oscillations ($\sim 10^{21}$ Hz). The advantage of above solid state structures over the vacuum is a much lower magnitude of ZB frequency, which greatly facilitates its experimental detection in these materials [12,14–16]. In [14] the coherent electron ZB had been shown experimentally to be triggered by initializing an ensemble of electrons in the same spin states. It had been probed in strained *n*-InGaAs as an ac-current at GHz frequencies. In [17, 18] a computer simulation of the damping of ZB oscillations for a wave packet of the Gaussian profile predicted theoretically in [11] had been performed. It should be noted that the study of ZB in Dirac crystals is also of practical importance. So in [19] a path for creating a nanoresonator based on a system of oscillatory circuits that exhibited the properties of an active load if external signal frequencies exceeded the ZB frequency had been outlined. In [20] similar systems had been used in microcircuits, which made it possible to simulate such relativistic quantum effects as the Klein paradox and ZB.

Presently, the problem of controlling the electron ZB in Dirac materials by means of external fields has become topical [21–23]. The possibility of ZB stabilization by a quantizing magnetic field had been shown in [24, 25]. The combination effect from simultaneous allowance of ZB in Dirac structures and an external HF electromagnetic (EM) field had been investigated in [21, 26, 27].

In [27] the so-called multi-mode ZB (electron oscillations induced by an HF electric field) had been studied for free graphene. The spectrum of such oscillations contained new frequencies equal to combinations of the monochromatic field frequency and the ZB frequency. However, the calculations in [27] had not been performed for arbitrary electron momenta: the momentum along the polarization line had been assumed zero. This does not correspond to the real situation, in which the momenta of charge carriers obey 2D statistics. Moreover, in some cases the ac-field amplitude had been assumed sufficiently small. It had allowed solving the equations of motion in the approximation linear in the ac-field amplitude. As a result, the multi-mode ZB spectrum contained only two new frequencies (besides ZB frequency). Below both the rotating wave approximation (RWA) and the approximation of high driving frequency (HDF) are used for calculations as in [27]. However, in contrast to [27] analytical calculations are performed for arbitrary ac-field amplitudes and in the case of using HDF for arbitrary electron momenta. For intensive fields the spectrum of the multi-mode ZB is shown to contain a series of new (compared to conventional ZB) frequencies, which are the combination of the ZB frequency and frequencies that are multiples of the pump field frequency. Among other things, the result is generalized to the case of a Hamiltonian model describing two independent Dirac points [8].

Effect of velocity rectification in monochromatic field

Let 2D Dirac crystal associated with *xy*-plane is subjected by the monochromatic EM radiation so that electric field oscillates along *Ox* axis. Spinor ψ describing the electron state in this case obeys

$$i\frac{\partial\psi}{\partial t}=\left(\Omega_1\hat{\sigma}_x+\Omega_2\hat{\sigma}_y\right)\psi+e\upsilon_{\mathrm{F}}A\left(t\right)\hat{\sigma}_x\psi, \tag{1}$$

where $\hat{\sigma}_{x,y,z}$ are Pauli matrices, $\mathbf{A}(t)$ is vector potential of ac field, $\Omega_1=\upsilon_{\mathrm{F}}p_x$, the form of the term Ω_2 is determined by the crystal model. For the conical model, for instance, one has $\Omega_2=\upsilon_{\mathrm{F}}p_y$. Further we use the model of 2D crystal with displaced Dirac points [8]:

$$\Omega_2=\frac{p_y^2}{2m}-\Delta, \tag{2}$$

and $\Delta > 0$. We note that the change in the sign of the parameter Δ leads to the transition between semi-metal and band insulator states. In the latter case, the crystal will be of semi-Dirac type. The time dependence of ac-field is assumed to be harmonic: $A(t) = (E_0/\omega)\cos(\omega t + \varphi_0)$. Here E_0 is amplitude of the electric field intensity, ω is its frequency and φ_0 is its initial phase. Electron ZB is shown below modifies the spectrum of electron velocity oscillations in the monochromatic ac-field. To investigate this modification the initial state in p-representation is assumed to be given by a delta-like wave function: $\psi_0 = \delta(\mathbf{p} - \mathbf{p}')\chi_0$, where χ_0 is eigenspinor of the matrix $\hat{\sigma}_s$ [27]: $\chi_0 = (1\ 0)^{\mathrm{T}}$. Let us note here the next peculiarity of the electron dynamics in Dirac crystals. If $\Omega_2 = 0$, then Eq. (1) admits the exact analytical solution

$$\psi\left(t\right)=e^{-i\left(\Omega_1 t+a_0\sin\left(\omega t+\varphi_0\right)\right)\hat{\sigma}_x}\psi_0, \tag{3}$$

where $a_0 = \upsilon_{\mathrm{F}}eE_0/\omega^2$. The components of quantum mechanical average velocity of electron which are calculated as the matrix elements $\upsilon_{x,y} = \upsilon_{\mathrm{F}}\langle\psi|\,\hat{\sigma}_{x,y,z}|\psi\rangle$ read

$$\upsilon_x=0,\upsilon_y=-\upsilon_{\mathrm{F}}\sin\left(\Omega_{\mathrm{ZB}}t+2a_0\sin\left(\omega t+\varphi_0\right)\right). \tag{4}$$

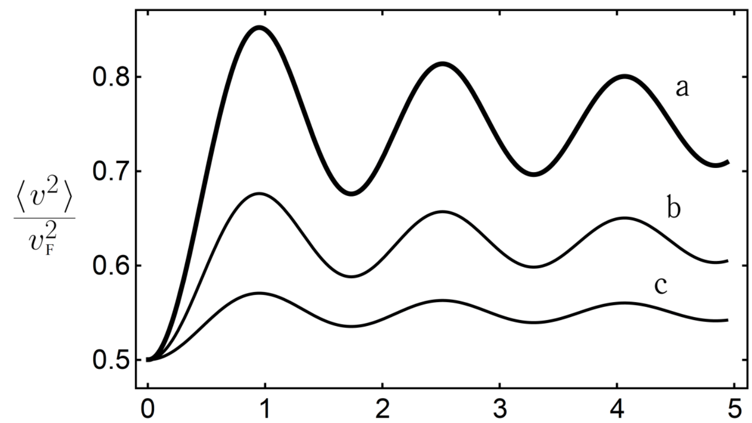

Fig. 1. Intensity of multi-mode Zitterbewegung $\langle\upsilon^2\rangle$ vs. ac-field amplitude: $\Omega_1 = 0$ (*a*); $\Omega_1 = \Omega_2$ (*b*) ; $\Omega_1 : \Omega_2=2 : 1$ (*c*)

Here Ω_{ZB} is ZB frequency in the absence of ac-field. There can be the next situation according to Eq. (4). If $\varphi_0 \neq s\pi$ and ZB frequency is multiples of ac-field frequency, $\Omega_{ZB}=k\omega$ (s and k are integers), then electron velocity acquires the stationary component which reads

$$\left\langle \upsilon_y \right\rangle_t = \left(-1\right)^k J_k\left(2a_0\right)\upsilon_{\mathrm{F}} \sin k\varphi_0, \tag{5}$$

where $J_k(x)$ is Bessel function of integer order. Particularly in the case when $\varphi_0 = \pi/2$ one can obtain $\left\langle \upsilon_y \right\rangle_t = \left(-1\right)^{k+1} J_{2k+1}\left(2a_0\right)\upsilon_{\mathrm{F}}$. Such a "velocity rectification" is the nonlinear effect related with the combination of two vibrations of electron in Dirac crystal: ZB existing in the absence of ac-field and forced vibrations arising due to the effect of ac-field.

Multi-mode ZB in HF electric field

To analyze the behavior of electron velocity at arbitrary values of Ω_2 it is convenient to use the unitary transformation by means of operator

$$\hat{U} = e^{i\Omega t\hat{\sigma}_0}, \tag{6}$$

where we have define $\hat{\sigma}_0 = \left(\Omega_1\hat{\sigma}_x + \Omega_2\hat{\sigma}_y\right)/\Omega$, $\Omega = \sqrt{\Omega_1^2 + \Omega_2^2}$. In [27] to study the nonlinear dynamics of Dirac electron within the HDF picture the solution of Eq. (1) had been limited by an approximation linear in the ac-field amplitude a_0. The unitary operator (6) used here differs from that used in [27] and allows one to obtain analytical results for arbitrary ac-field amplitudes. Having put in Eq. (1) $\psi = \hat{U}^{+}\chi$, $\hat{\Sigma}_{x,y,z}\left(t\right) = \hat{U}\hat{\sigma}_{x,y,z}\hat{U}^{+}$ and $\varphi_0 = 0$, we arrive at

$$\frac{\partial\chi}{\partial t} = -i\omega a_0 \cos\omega t\hat{\Sigma}_x\left(t\right)\chi. \tag{7}$$

Now the condition $\omega \gg \Omega$ (HDF approximation) is assumed to be performed. Then it is easy to verify that the spinor

$$\chi\left(t\right) = e^{-ia_0 \sin\omega t\hat{\Sigma}_x(t)}\chi_0 \tag{8}$$

is the solution of Eq. (7). Indeed, terms, which are the result of differentiation of the spinor $\hat{\Sigma}_x\left(t\right)\chi_0$ can be neglected, because of they will contain as a multiplier the frequencies which are much less than ω. To prove it let us write the time-derivative for spinor (8) explicitly:

$$\frac{\partial\chi}{\partial t} = -i\omega a_0\left(\cos\omega t\hat{\Sigma}_x + \frac{1}{\omega}\sin\omega t\frac{\partial\hat{\Sigma}_x}{\partial t}\right)\chi. \tag{9}$$

Using the definition (6) one can find that $\dot{\hat{\Sigma}}_x = \Omega_2\hat{\Sigma}_z$. After substitution of latter derivative into Eq. (9) and neglecting of the term containing Ω_2/ω ($\Omega_2 \leq \Omega << \omega$) we arrive at Eq. (8). The average quantum mechanical velocity $\upsilon_{x,y} = \upsilon_{\mathrm{F}}\left\langle\chi\left|\hat{\Sigma}_{x,y}\right|\chi\right\rangle$ is derived by means of spinor (8). After some algebra one obtains

$$\upsilon_x = \frac{\upsilon_{\mathrm{F}}\Omega_2}{\Omega}\sin 2\Omega t, \tag{10}$$

$$\upsilon_y = -\frac{\upsilon_{\mathrm{F}}\Omega_1}{\Omega}\cos\left(2a_0\sin\omega t\right)\sin 2\Omega t - \upsilon_{\mathrm{F}}\sin\left(2a_0\sin\omega t\right)\cos 2\Omega t. \tag{11}$$

As expected the velocity vibrations, according to Eq. (11), are not harmonic. To analyze the spectral composition of these vibrations, we expand the right side of Eq. (11) into a Fourier series:

$$\begin{aligned}\upsilon_y = &-\frac{\upsilon_{\mathrm{F}}\Omega_1}{\Omega}J_0\left(2a_0\right)\sin 2\Omega t + \frac{\upsilon_{\mathrm{F}}\Omega_1}{\Omega}\sum_{n=1}^{\infty}J_{2n}\left(2a_0\right)\left(\sin 2\left(n\omega-\Omega\right)t - \sin 2\left(n\omega+\Omega\right)t\right) - \\ &-\upsilon_{\mathrm{F}}\sum_{n=0}^{\infty}J_{2n+1}\left(2a_0\right)\left(\sin\left(\left(2n+1\right)\omega+2\Omega\right)t + \sin\left(\left(2n+1\right)\omega-2\Omega\right)t\right).\end{aligned} \tag{12}$$

Thus, the spectrum of electron velocity vibrations contains, as the main frequency, the ZB frequency equal to 2Ω, and additional frequencies $n\omega\pm2\Omega$, where n is an integer. This type of motion of Dirac electron in a monochromatic field has been called as multi-mode ZB in [27]. If $p_x = 0$ and $a_0 \ll 1$, then, as expected, Eqs. (10) and (12) are transformed into the corresponding formulas from [27]. The multi-mode ZB intensity is proportional to the time-averaged square of the electron velocity $\left\langle \upsilon^2 \right\rangle = \left\langle \upsilon_x^2 \right\rangle + \left\langle \upsilon_y^2 \right\rangle$ [27]. Using Eqs. (10) and (12), we find

$$\left\langle \upsilon^2 \right\rangle = \upsilon_F^2 \left(\frac{\Omega_2^2}{2\Omega^2} + \frac{\Omega_1^2}{2\Omega^2} \left(J_0^2\left(2a_0\right) + 2\sum_{n=1}^{\infty} J_{2n}^2\left(2a_0\right) \right) + \sum_{n=0}^{\infty} J_{2n+1}^2\left(2a_0\right) \right). \tag{13}$$

The dependence of $\langle \upsilon^2 \rangle$ on the dimensionless amplitude of ac-field a_0 plotted by Eq. (13) is shown in Fig. 1 for different values of Ω_1 and Ω_2. If $\Omega_2 = 0$ then $\langle \upsilon^2 \rangle$ does not depend on the amplitude a_0 and is equal to $\upsilon_F^2 / 2$.

Rabi frequency

In this section as in [27] we put $p_x = 0$. However the model (2) is used here instead of conical model of Hamiltonian. RWA allows us to find the solution of Eq. (1) in the case $|2|\Omega_2| - \omega|$†ω. The components oscillating with frequency $2|\Omega_2| + \omega$ are neglected within RWA. In this situation spectrum of vibrations will still contain three frequencies: Ω_R, $\Omega_R \pm \omega$, where Ω_R is so called Rabi frequency, which reads

$$\Omega_R = \sqrt{\left(2\left|\Omega_2\right| - \omega\right)^2 + \upsilon_F^2 p_0^2}. \tag{14}$$

Here $p_0 = eE_0/\omega$. Rabi frequency is seen from (14) to be determined by three structure parameters υ_F, m and Δ instead one parameter υ_F as it was in conical model [27]. In addition the anisotropy of the Hamiltonian model [8] which takes into account two Dirac points leads to the fact that the character of the dependence of the Rabi frequency on the amplitude of ac-field will be determined by the direction of the polarization of this field in the 2D crystal plane. Now we make sure of this clearly. To do this we change the direction of the field polarization so that it oscillates along the Oy axis. Then instead of Eq. (1) one should write

$$i\frac{\partial\Psi}{\partial t} = \Omega_1 \hat{\sigma}_x \psi + \tilde{\Omega}_2 \hat{\sigma}_y \psi + \omega\left(\frac{p_0^2}{4m\omega}\cos 2\omega t + \frac{p_y p_0}{m\omega}\cos\omega t \right)\hat{\sigma}_y \psi, \tag{15}$$

where we define $\tilde{\Omega}_2 = \Omega_2 + p_0^2/4m$. Further we put $\tilde{\Omega}_2 = 0$. The latter can be reached if $\Delta > 0$ and $eE_0 < 2\omega\sqrt{m\Delta}$. Then after transformations by means of operator $\hat{S} = e^{i\Omega_1 t\hat{\sigma}_x}$ we arrive at

$$\frac{\partial\chi}{\partial t} = -i\omega\left(a_1\cos\omega t + a_2\cos 2\omega t\right)\hat{\Xi}_y \chi. \tag{16}$$

Here $\hat{\Xi}_y = \hat{S}\hat{\sigma}_y\hat{S}^+$, $a_1 = \pm q_0 p_0 / m\omega$, $a_2 = p_0^2/4m\omega$, $q_0 = \sqrt{2m\Delta - p_0^2/2}$. To solve Eq. (16) we use RWA, which can be applied in two cases: (a) $|2|\Omega_1| - \omega| \ll \omega$ or (b) $2||\Omega_1| - \omega| \ll \omega$. In the case (a), we leave in Eq. (16) only terms oscillates with a frequency $2|\Omega_1| - \omega$. As a result we have $\left(a_1\cos\omega t + a_2\cos 2\omega t\right)\hat{\Xi}_y \approx \left(a_1/2\right)e^{i\left(2|\Omega_1| - \omega\right)t\hat{\sigma}_x}\hat{\sigma}_y$. So instead of Eq. (16) one obtains

$$\frac{\partial\chi}{\partial t} = \frac{i\omega a_1}{2} e^{i\left(2|\Omega_1| - \omega\right)t\hat{\sigma}_x}\hat{\sigma}_y \chi. \tag{17}$$

After some transformations we write

$$\frac{\partial^2\chi}{\partial t^2} - i\left(2\left|\Omega_1\right| - \omega\right)\hat{\sigma}_x \frac{\partial\chi}{\partial t} + \frac{\omega^2 a_1^2}{4}\chi = 0. \tag{18}$$

Particular solutions of Eq. (18) have the form $\chi_{\pm}(t) = e^{-(i/2)(\omega - 2|\Omega_1| \pm \Omega_R) t \hat{\sigma}_x} \chi_0$, where Rabi frequency reads

$$\Omega_R = \sqrt{\left(2|\Omega_1| - \omega\right)^2 + \frac{2\Delta p_0^2}{m}\left(1 - \frac{p_0^2}{4m\Delta}\right)}, \tag{19}$$

In the case $2\|\Omega_1| - \omega| \ll \omega$ only terms oscillates with a frequency $2(|\Omega_1| - \omega)$ should be leaved in Eq. (16). After similar transformations, one obtains for the Rabi frequency the expression

$$\Omega_R = \sqrt{4\left(|\Omega_1| - \omega\right)^2 + \frac{p_0^4}{16m^2}}. \tag{20}$$

The dependence of Rabi frequency on amplitude $p_0 = eE_0/\omega$ is seen from Eqs. (14), (19) and (20), to be different for different polarizations of ac-field. It is explained by the anisotropy of the spectrum of 2D Dirac crystal with the Hamiltonian [8].

Conclusion

We have considered the nonlinear dynamics of an electron in 2D Dirac crystal placed in AC electric field of monochromatic radiation with frequency ω. In contrast to [27] the model of Hamiltonian [8] used in the above calculations has taken into account the presence of two independent Dirac points and has been characterized by significant anisotropy. Taking into account ZB (oscillations of free Dirac electron) has led to the modification of the spectrum of nonlinear oscillations of an electron in the external ac-field. In HDF approximation, when the external field frequency is much higher than the ZB frequency Ω_{ZB}, this spectrum contains combinations $n\omega \pm 2\Omega_{ZB}$ (n is an integer). It should be mentioned that the multi-mode dynamics of Dirac electron in monochromatic field had been studied earlier in [27], where three frequencies in the spectrum of electron oscillations had been predicted within HDF approximation: Ω_{ZB} and $\omega \pm 2\Omega_{ZB}$. However, stated in [27] theory had been limited by both 1D motion of an electron and linear approximation of the amplitude of AC field. Here in contrast to [27] we have studied the case of arbitrary directions of the quasi-momentum and arbitrary amplitudes of HF radiation. As a result, the functional dependence of the multi-mode ZB intensity on the amplitude of ac-field a_0 has been derived (Fig. 1). Moreover, Eq. (12) allows analytical calculation of dependence of arbitrary n-harmonics of multimode ZB on a_0.

The spectrum of electron oscillations obtained within RWA, when the frequency of the external ac-field is comparable with ZB frequency, contains, as in [27], three frequencies: Ω_R, $\Omega_R \pm \omega$ (Ω_R is Rabi frequency). However, in contrast to [27], the dependence of Ω_R on the amplitude of EM radiation is determined by the direction of its polarization (see Eqs. (14), (19) and (20)). The latter is related to the anisotropy of the Hamiltonian [8] used in the calculations. At the end, we point out the possibility of the appearance of a constant term of electron velocity in 2D Dirac crystal in the field of monochromatic radiation. To this end, it is necessary that ZB frequency be a multiple of the frequency of ac-field. Moreover, according to Eq. (5), the value of such a "rectified" velocity is determined by the amplitude of this field.

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