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Multi-mode dynamics of electrons in a Dirac crystal in the field of monochromatic radiation

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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 changing 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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Introduction

The discovery of new types of 2D-crystals, comprising a group of so-called Dirac materials (graphene, germanene, silicene, etc.), as well as the study of their electrodynamic properties has determined, in fact, the development of that part of solid-state physics, which stands at the interface between the condensed state theory and high energy physics. The point is that the relativistic form of the equations for electronic states in hexagonal 2D lattices makes graphene-like materials a convenient platform for studying the effects of quantum electrodynamics [1–4]. The uniqueness of the above materials can be explained by the presence of terms in the quantum equation for electronic states that connect the charge carrier momentum with its pseudo-spin degree of freedom. Examples of such connection manifestations are topological phase transitions [5–10] of the „half-metal-insulator“ [7,11,12] and „Dirac-half-dirac material“ [13,14] type, as well as the Zitterbewegung (ZB) effect — rapid velocity oscillations of a free (pseudo)relativistic electron resulting from the states interference with positive and negative energies.

The ZB possibility for electrons in crystals described by a pseudo-relativistic Hamiltonian is shown theoretically in [15–18]. As for the experimental realization of ZB, due to the high frequency of the corresponding electron oscillations in the vacuum ($\sim 10^{21}$ Hz), the observation of this effect is very difficult. The advantage of Dirac structures over vacuum, however, is the much lower ZB frequency, which makes it much easier to detect experimentally in these materials [19–21]. A computer simulation of the ZB oscillation attenuation for the Gaussian wave packet predicted earlier theoretically [17] was performed in 22,23. It is worth noting that the ZB study in Dirac crystals is also of applied importance. Thus, in [24], the way to create a nano-resonator based on a system of oscillating circuits exhibiting active load properties at external signal frequencies higher than the ZB frequency is outlined. In [25], similar systems were used in microcircuits which allowed to simulate such relativistic quantum effects as the Klein and ZB paradox.

Recently, the issue of controlling the electronic ZB in Dirac materials due to external force fields has become urgent. In particularly, [26–28] proposes a solution to the ZB attenuation problem for an electron wave packet of finite width. In [29,30] the possibility of ZB stabilizing by a quantized magnetic field is shown. The combinational effect of simultaneous accounting for ZB in Dirac structures and an external high-frequency (HF) electromagnetic (EM) field was investigated in [26,31,32].

In work [32], for free graphene, the so-called multimode ZB — electron oscillations induced by the HF electric field were studied. The spectrum of such oscillations contained new frequencies equal to combinations of the monochromatic field frequency and ZB frequency. However, in [32], the calculations were not performed for arbitrary electron pulses: the pulse along the polarization line was assumed to be zero. This does not correspond to the real situation, in which the charge carrier pulses obey 2D statistics. In addition, in some cases, the field amplitude was assumed to be small enough to allow the equations of motion to be solved in the linear field amplitude approximation. As a result, the spectrum of multimode ZB contained only two new frequencies. Below, as in [32], the (1) rotating wave approximation (RWA) and (2) high driving frequency (HDF) are used for calculations. In contrast to [32], the analytical calculations were performed for arbitrary amplitudes of the alternating field and in the case of the HDF for arbitrary electron pulses. It is shown that for strong fields, the spectrum of multimode ZB contains a series of new (compared to conventional ZB) frequencies, which are a combination of the ZB frequency and frequencies that are multiples of the pumping field frequency. Among other things, the result is generalized to the case of a Hamiltonian model describing two independent Dirac points [13].

The constant component of electron velocity in a monochromatic field

Let a Dirac 2D crystal, to which we will connect the xy plane, be placed in the field of monochromatic EM radiation propagating along Oz so that its electric component oscillates along Ox. In the future, we will neglect the coordinate dependence of the electric field strength of the wave, considering that the length of the latter is much greater than the thickness of the material in question. Spinor ψ, describing the electron state in such a situation, satisfies the equation

$$i\,\frac{\partial\psi}{\partial t} = (\Omega_1\hat{\sigma}_x + \Omega_2\hat{\sigma}_y)\psi + \omega a(t)\hat{\sigma}_x\psi, \tag{1}$$

where $\hat{\sigma}_{x,y,z}$ — Pauli matrices, ω — frequency of the alternating field, $\hbar\Omega_1 = \upsilon_F p_x$, and the form of the summand $\hbar\Omega_2$ will be determined by the crystal model. For example, for the conic spectrum model $\hbar\Omega_1 = \upsilon_F p_y$. In the following, we use the model of a 2D crystal with displaced Dirac points [13]:

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

with $\Delta > 0$. Note, that changing the sign of the parameter Δ to the opposite means the transition from the semi-metallic state to the state of a zone insulator. In the latter case, the crystal will be of the half-Dirac type.

We assume that the time dependence of the HF signal is harmonic: $a(t) = a_0\cos(\omega t + \varphi_0)$. Here, $a_0 = \upsilon_F p_0/\hbar\omega$, $p_0 = eE_0/\omega$, E_0 — the amplitude of the electric field strength, φ_0 — the initial phase. In addition, we consider that the initial state in the momentum representation is described by a spinor

$$\psi_0(\mathbf{p}) = \frac{f(\mathbf{p}-\mathbf{p}')}{\sqrt{C_1^2 + C_2^2}}\,\chi_0, \tag{3}$$

where $f(\mathbf{p}-\mathbf{p}')$ — is the normalized function specifying the profile of the wave packet with initial momentum $\mathbf{p}'$, $\chi_0 = (C_1\,C_2)^T$, and components C_1 and C_2 define the orientation of the pseudo-spin [18,23,33]. To study exactly the modification due to ZB of the spectral composition of the electron velocity oscillations in the monochromatic force field, rather than the temporal evolution of the wave packet as $f(\mathbf{p})$, it is sufficient to choose the delta profile [32]: $f(\mathbf{p}) = \delta(\mathbf{p})$. Choosing as the initial function $f(\mathbf{p})$ a Gaussian wave packet of finite width, which is usually dealt with in works [15,18,23,33–36], will lead to the standard situation of electronic oscillation attenuation [17].

If $\Omega_2 = 0$, then equation (1) has an exact analytical solution

$$\psi(t) = e^{-i(\Omega_1 t + a_0\sin(\omega t+\varphi_0))\hat{\sigma}_x}\psi_0. \tag{4}$$

For certainty, we fix $C_1 = 1$, and the parameter C_2 will be considered arbitrary, $C_2 = \alpha$. For example, the values $\alpha = 1$, $\alpha = i$ and $\alpha = 0$ describe states with pseudo-spin orientation along the axes Ox, Oy and Oz, respectively. The components of the average quantum mechanical speed of the electron calculated as matrix elements $\upsilon_{x,y} = \upsilon_F\langle\psi|\hat{\sigma}_{x,y}|\psi\rangle$, are equal

$$\upsilon_x = \frac{2\upsilon_F \mathrm{Re}\alpha}{1+|\alpha|^2},$$

$$\upsilon_y = 2\upsilon_F\frac{\mathrm{Im}\alpha}{1+|\alpha|^2}\cos\big(\Omega_{ZB}t + b(t)\big) - \upsilon_F\frac{1-|\alpha|^2}{1+|\alpha|^2}\sin\big(\Omega_{ZB}t + b(t)\big), \tag{5}$$

where the $\Omega_{ZB} = 2\Omega_1$ — frequency of velocity oscillations in the absence of a variable field (ZB frequency), $b(t) = 2a_0\sin(\omega t + \varphi_0)$. In particular, for $\alpha = 0$, we have

$$\upsilon_x = 0,\ \ \upsilon_y = -\upsilon_F\sin\big(\Omega_{ZB}t + 2a_0\sin(\omega t+\varphi_0)\big). \tag{6}$$

According to (6), the following situation is possible. If $\varphi_0 \neq s\pi$, and the frequency of ZB is a multiple of the AC field frequency, $\Omega_{ZB} = k\omega$ (s and k — integers), then the electron speed has a constant component equal to

$$\langle\upsilon_y\rangle_t = (-1)^k J_k(2a_0)\upsilon_F\sin k\varphi_0. \tag{7}$$

Here, $J_k(x)$ – is a Bessel function of k-th order. In particular, if $\varphi_0 = \pi/2$, then the constant velocity component is non-zero only when the ratio Ω_{ZB}/ω is an odd number: $\Omega_{ZB} = (2k+1)\omega$. Wherein $\langle\upsilon_y\rangle_t = (-1)^{k+1}J_{2k+1}(2a_0)\upsilon_F$. Such „rectification“ of the velocity is caused by a combination of two vibrational movements of the electron in a Dirac crystal: ZB vibrations, which take place in the absence of the field, and forced vibrations, arising due to the force action from the alternating electric field.

Multimode ZB in HF electric field

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

$$\hat{U} = e^{i\Omega t\hat{\sigma}_0}, \quad (8)$$

with the designation

$$\hat{\sigma}_0 = \frac{\Omega_1\hat{\sigma}_x + \Omega_2\hat{\sigma}_y}{\Omega},\ \ \Omega = \sqrt{\Omega_1^2 + \Omega_2^2}.$$

In [32], to study the nonlinear dynamics of the Dirac electron within HDF, the solution to equation (1) was limited to the a_0 approximation linear in field amplitude. The unitary transformation operator used here (8) differs from the analogous operator used in [32] and allows us to obtain analytical results for arbitrary HF field amplitudes. By putting in (1) $\psi = \hat{U}^+\chi$ and $\hat{\Sigma}_{x,y,z}(t) = \hat{U}\hat{\sigma}_{x,y,z}\hat{U}^+$, $\varphi_0 = 0$, we will come, after some transformations, to the following equation:

$$\frac{\partial\chi}{\partial t} = -i\omega a_0 \cos\omega t\hat{\Sigma}_x(t)\chi. \quad (9)$$

Let us suppose that the following condition is satisfied: $\omega \gg \Omega$ (HDF approximation). Then it is not difficult to see that the spinor

$$\chi(t) = e^{-ia_0 \sin\omega t\hat{\Sigma}_x(t)}\chi_0 \quad (10)$$

is a solution to equation (9). Indeed, the terms equal to the result of the spinor differentiation $\hat{\Sigma}_x(t)\chi_0$ can be neglected, since the latter will contain as a multiplier low compared to ω frequencies. With the help of spinor (10), let us calculate the average quantum mechanical speed of the electron:

$$\upsilon_{x,y} = \upsilon_F\langle\chi|\hat{\Sigma}_{x,y}|\chi\rangle. \quad (11)$$

For certainty, let us consider the quite common case in the literature when the initial pseudo-spin is oriented perpendicular to the 2D-crystal plane, i.e., $\chi_0 = (1\,0)^T$ [15,18,23,32–36]. After substituting (10) into (11) and some transformations, we obtain

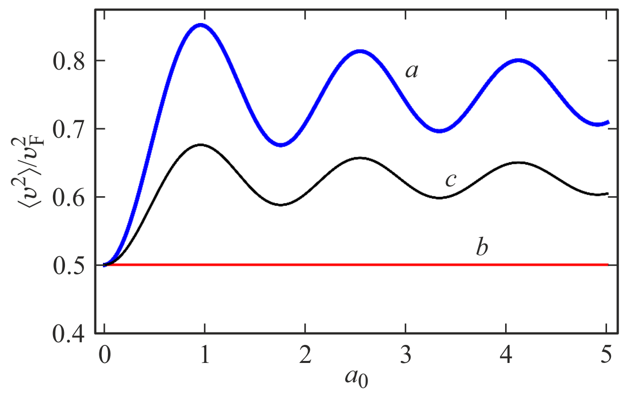
$$\upsilon_x = \frac{\upsilon_F\Omega_2}{\Omega}\sin 2\Omega t, \quad (12)$$

$$\upsilon_y = -\frac{\upsilon_F\Omega_1}{\Omega}\cos(2a_0\sin\omega t)\sin 2\Omega t$$
$$- \upsilon_F\sin(2a_0\sin\omega t)\cos 2\Omega t. \quad (13)$$

As one would expect, the velocity fluctuations, according to (13), are not harmonic.

To analyze the spectral composition of these oscillations, we decompose function (13) into a Fourier series:

$$\upsilon_y = -\frac{\upsilon_F\Omega_1}{\Omega}J_0(2a_0)\sin 2\Omega t + \frac{\upsilon_F\Omega_1}{\Omega}$$
$$\times\sum_{n=1}^{\infty}J_{2n}(2a_0)\big(\sin 2(n\omega - \Omega)t - \sin 2(n\omega + \Omega)t\big)$$
$$-\upsilon_F\sum_{n=0}^{\infty}J_{2n+1}(2a_0)\big(\sin((2n+1)\omega + 2\Omega)t$$
$$+\sin((2n+1)\omega - 2\Omega)t\big). \quad (14)$$



Dependence of $\langle\upsilon^2\rangle$ on the amplitude of the RF electric field. a — $\Omega_1 = 0$; b — $\Omega_2 = 0$; c — $\Omega_1 = \Omega_2$.

Thus, the spectrum of electron velocity oscillations contains as the main frequency ZB, equal to 2Ω, and additional frequencies $n\omega \pm 2\Omega$, where n — an integer. This type of motion of a Dirac electron in a monochromatic field in [32] is called multi-mode ZB. If p_x and $a_0 \ll 1$, then, as one would expect, expressions (12) and (14) pass into the corresponding formulas from [32]. The intensity of multimode ZB is proportional to the time-averaged square of the electron velocity $\langle\upsilon^2\rangle = \langle\upsilon_x^2\rangle + \langle\upsilon_y^2\rangle$ [32]. Using formulas (12) and (14), we find

$$\langle\upsilon^2\rangle = \upsilon_F^2\bigg(\frac{\Omega_2^2}{2\Omega^2} + \frac{\Omega_1^2}{2\Omega^2}\Big(J_0^2(2a_0) + 2\sum_{n=1}^{\infty}J_{2n}^2(2a_0)\Big)$$
$$+\sum_{n=0}^{\infty}J_{2n+1}^2(2a_0)\bigg). \quad (15)$$

The dependence of $\langle\upsilon^2\rangle$ on the dimensionless amplitude of the HF field a_0, constructed by the formula (15), is shown in the figure for different values Ω_1 and Ω_2. If $\Omega_2 = 0$, then the value of $\langle\upsilon^2\rangle$ is independent of amplitude a_0 and equal to $\upsilon_F^2/2$.

As can be seen, the multimode effect appears only for the velocity component υ_y, which is due to the chosen orientation of the plane of polarization of the incident radiation. We should expect that in the case of an elliptically polarized wave, for example, the multimode effect will be observed in both components of the average velocity.

It is not difficult to obtain the average velocity for other initial spinor structures as well. Below, there are the results for the υ_y component only. Thus, in the case $\chi_0 = (1\,i)^T$, corresponding to the orientation of the initial pseudo-spin along Ox, we have

$$\upsilon_y = \frac{\upsilon_F\Omega_2}{\Omega}\bigg(\frac{\Omega_1}{\Omega}(1 - \cos 2\Omega t)\cos b_0 + \sin 2\Omega t\sin b_0\bigg). \quad (16)$$

Here, b_0 — the oscillating function $b(t)$ appearing in (5), at $\varphi_0 = 0$. If $\chi_0 = (1\,i)^T$, which corresponds to the initial orientation of the pseudo-spin along Oy, then

$$\upsilon_y = \frac{\upsilon_F}{\Omega^2}(\Omega_2^2 + \Omega_1^2 \cos 2\Omega t)\cos b_0 - \frac{\upsilon_F \Omega_1}{\Omega}\sin 2\Omega t \sin b_0. \quad (17)$$

Rabi frequency

Here, as in [32], we will put $p_x = 0$, but instead of the conic Hamiltonian model, we will use the model (2). The RWA approximation allows to find solutions to equation (1) under the condition $|2|\Omega_2| - \omega| \ll \omega$. The RWA frames neglect the terms oscillating with frequency $2|\Omega_2| + \omega$. In this case, the spectrum of velocity oscillations will still contain three frequencies: Ω_R, $\Omega_R \pm \omega$, where Ω_R — the so-called Rabi frequency, which has the form

$$\Omega_R = \sqrt{(2|\Omega_2| - \omega)^2 + \frac{\upsilon_F^2 p_0^2}{\hbar^2}}. \quad (18)$$

As can be seen from (18), unlike [32] the Rabi (18) frequency is determined by three crystal structure parameters υ_F, m and Δ instead of one parameter υ_F. In addition, the anisotropy of the Hamiltonian [13] model, which considers 2 dirac points, leads to the fact that the character of the Rabi frequency dependence on the AC field amplitude will be determined by the polarization direction of this field in the 2D-crystal plane. Let us make sure of that explicitly. To do this, change the direction of polarization of the field so that it oscillates along the Oy axis. Then instead of (1), we should write

$$i\frac{\partial\psi}{\partial t} = \Omega_1\hat{\sigma}_x\psi + \tilde{\Omega}_2\hat{\sigma}_y\psi + \omega\left(\frac{p_0^2}{4m\hbar\omega}\cos 2\omega t + \frac{p_y p_0}{m\hbar\omega}\cos\omega t\right)\hat{\sigma}_y\psi, \quad (19)$$

with the designation

$$\tilde{\Omega}_2 = \Omega_2 + \frac{p_0^2}{4m}. \quad (20)$$

Next, consider that $\tilde{\Omega}_2 = 0$, which can be achieved if $\Delta > 0$ and $eE_0 < 2\omega\sqrt{m\Delta}$. Then, after the transformation with the operator

$$\hat{S} = e^{i\Omega_1 t\hat{\sigma}_x} \quad (21)$$

write instead (19)

$$\frac{\partial\chi}{\partial t} = -i\omega(a_1\cos\omega t + a_2\cos 2\omega t)\hat{\Xi}_y\chi. \quad (22)$$

Here, $\hat{\Xi}_y = \hat{S}\hat{\sigma}_y\hat{S}^+$, $a_1 = \pm q_0 p_0/m\hbar\omega$, $a_2 = p_0^2/4m\hbar\omega$, $q_0 = \sqrt{2m\Delta - p_0^2/2}$. To solve equation (22), apply the RWA method. The latter is justified in two cases: (a) $|2|\Omega_1| - \omega| \ll \omega$ or (b) $2|\Omega_1| - \omega| \ll \omega$. In the first case, we leave in (22) only those terms that oscillate with frequency $2||\Omega_1| - \omega$. As a result, we arrive at the following ratio:

$$(a_1\cos\omega t + a_2\cos 2\omega t)\hat{\Xi}_y \approx \frac{a_1}{2}e^{i(2|\Omega_1| - \omega)t\hat{\sigma}_x}\hat{\sigma}_y.$$

Then, instead of (22) we get

$$\frac{\partial\chi}{\partial t} = -\frac{i\omega a_1}{2}e^{i(2|\Omega_1| - \omega)t\hat{\sigma}_x}\hat{\sigma}_y\chi. \quad (23)$$

After some transformations, we write

$$\frac{\partial^2\chi}{\partial t^2} - i(2|\Omega_1| - \omega)\hat{\sigma}_x\frac{\partial\chi}{\partial t} + \frac{\omega^2 a_1^2}{4}\chi = 0. \quad (24)$$

Partial solutions to equation (24) have the form

$$\chi_\pm(t) = e^{-\frac{i}{2}(\omega - 2|\Omega_1| \pm \Omega_R)t\hat{\sigma}_x}\chi_0, \quad (25)$$

where the Rabi frequency

$$\Omega_R = \sqrt{(2|\Omega_1| - \omega)^2 + \frac{2\Delta p_0^2}{m\hbar^2}\left(1 - \frac{p_0^2}{4m\Delta}\right)}. \quad (26)$$

In the case of $2||\Omega_1| - \omega| \ll \omega$ in equation (22), the terms oscillating with frequency $2|\Omega_1| - 2\omega$ should be left out. As a result, after similar transformations, we obtain for the Rabi frequency

$$\Omega_R = \sqrt{4(|\Omega_1| - \omega)^2 + \frac{p_0^4}{16m^2\hbar^2}}. \quad (27)$$

As can be seen from (18), (26) and (27), the functional dependence of the Rabi frequency on the HF field amplitude ($p_0 = eE_0/\omega$) appears to be different for different polarizations of this field, which is explained by the anisotropy of the Dirac crystal spectrum with the Hamiltonian [13].

Conclusion

The nonlinear dynamics of an electron in a 2D Dirac crystal placed in an alternating electric field of monochromatic radiation of frequency ω are considered above. The model Hamiltonian used in the calculations [13], in contrast to [32], took into account the presence of 2 independent Dirac points and was characterized by substantial anisotropy. Taking into account the ZB — phenomenon of free Dirac electron oscillations —leads to a modification of the spectrum of nonlinear electron oscillations in an external HF force field. In the HDF approximation, when the frequency of the external field is much greater than the frequency of ZB, this spectrum contains combinations of $n\omega \pm 2\Omega$, where n — an integer, 2Ω —ZB frequency. It is worth mentioning that the multi-mode dynamics of the Dirac electron in a monochromatic field was studied earlier in [32], where three frequencies in the spectrum of electron oscillations were reported in the HDF: 2Ω and $\omega \pm 2\Omega$.

However, the theory built in [32] was limited to one-dimensional electron motion and linear in the amplitude of the HF field approximation. In the present work, in contrast to [32], the case of arbitrary directions of quasi-pulse and arbitrary amplitudes of HF radiation is investigated. As a result, a functional dependence of the intensity of multimode ZB on the amplitude of the HF field a_0 is obtained (figure). In addition, formula (14) allows to find the dependence on a_0 of the amplitude of an arbitrary nth harmonic of multimode ZB.

The spectrum of electron oscillations obtained in the framework of RWA, when the external field frequency is comparable with the ZB frequency, contains, as well as in [32], three frequencies: Ω_R, $\Omega_R \pm \omega$, where Ω_R — the Rabi frequency. However, unlike [32], the frequency dependence of Ω_R on the amplitude of EM radiation is determined by the direction of its polarization (formulas (18), (26) and (27)). The latter is due to the anisotropy of the Hamiltonian used in the calculations [13].

In conclusion, let us point out the possibility of the appearance of a constant velocity component in the electron of a 2D-dirac crystal in the field of monochromatic radiation. This requires that the frequency of ZB be a multiple of the frequency of the alternating electric field. And, according to formula (7), the value „of the rectified velocity“ is determined by the amplitude of this field.

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Conflict of interest

The authors declare that they have no conflict of interest.

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