Nonperturbative kinetic description of e-h excitations in graphene due a strong time-dependent electric field

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1. **Kinetic equation**
2. **e-h excitations in graphene**
3. **From linear to "circular" polarization**
4. **Residual currents**
5. **Summary**

1.Kinetic equation

Low-energy model for grapfene determined by the dispersion relation in the vicinity of the Dirac points in momentum space:

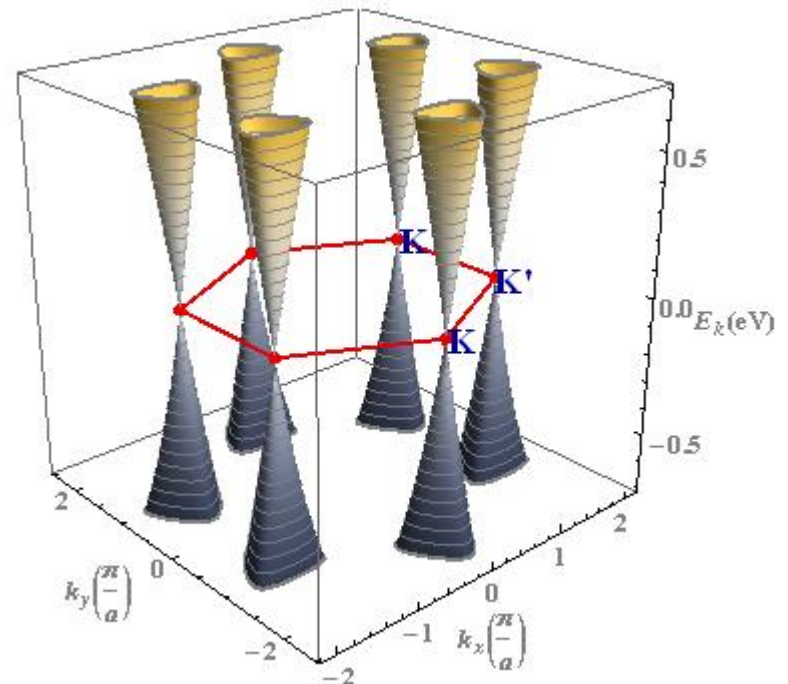$$\varepsilon(\vec{p}, t) = v_F \sqrt{p^2} = v_F \sqrt{(p^1)^2 + (p^2)^2}.$$

Here v_F - Fermi velocity,

p^i **- components of the quasiparticle momentum.**

For QED 3+1:
S.M. Schmidt, D. Blaschke, G. Reopke, S.A. Smolyansky, A.V. Prozorkevich and V.D. Toneev,
Int. J. Mod. Phys. E7, p.709 (1998)

The Hamiltonian of the low-energy model

$$H(t) = v_F \int d^2x \, \Psi^\dagger(\vec{x}, t) \hat{\vec{P}} \vec{\sigma} \Psi(\vec{x}, t)$$

and the equation of motion

$$i\hbar \dot{\Psi}(\vec{x}, t) = v_F \hat{\vec{P}} \vec{\sigma} \Psi(\vec{x}, t)$$

where $\hat{P}_k = -i\hbar\nabla_k - (e/c)A_k(t)$, σ_k **is the Pauli matrix.**

Two component electric field in the Hamilton gauge with arbitrary time dependence

$$A^k(t) = \left(0, A^1(t), A^2(t)\right)$$

We fulfill transition in the momentum representation and after that to the quasiparticle representation with help of unitary transformation with the matrix

$$U(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} \exp(-i\varkappa/2) & \exp(-i\varkappa/2) \\ \exp(i\varkappa/2) & -\exp(i\varkappa/2) \end{pmatrix}$$

where the definition is used $\tan\varkappa = P^2/P^1$ **and** $P^k = p^k - (e/c)A^k(t)$.

(B.Dora and R.Moessner, Phys. Rev. B <u>81</u>, 165431 (2010))

The Hamiltonian in the quasiparticle representation is diagonal and has the form:

$$H(t) = \int \frac{d^2 p}{(2\pi\hbar)^2} \varepsilon(\vec{p}, t) \left[a^\dagger(\vec{p}, t) a(\vec{p}, t) - b(-\vec{p}, t) b^\dagger(-\vec{p}, t) \right]$$

and the corresponding equations of motion

$$\dot{a}(\vec{p}, t) = \frac{i}{\hbar} \left[H(t), a(\vec{p}, t) \right] - \frac{i}{2} \lambda(\vec{p}, t) b^+(-\vec{p}, t)$$

$$\dot{b}(\vec{p}, t) = \frac{i}{\hbar} \left[H(t), b(-\vec{p}, t) \right] + \frac{i}{2} \lambda(\vec{p}, t) a^+(\vec{p}, t)$$

Where the amplitude of the transition between states is

$$\lambda(\vec{p}, t) = \frac{e v_F^2 [E_1 P_2 - E_2 P_1]}{\varepsilon^2(\vec{p}, t)}$$

The eigenvalues of Hamiltonian (energy of quasiparticles) are

$$\varepsilon(\vec{p}, t) = v_F \sqrt{P^2} = v_F \sqrt{(P^1)^2 + (P^2)^2}$$

In this representation the distribution functions of the electrons and holes is

$$f^e(\vec{p}, t) = \langle \text{in}|a^+(\vec{p}, t)a(\vec{p}, t)|\text{in}\rangle,$$

$$f^h(\vec{p}, t) = \langle \text{in}|b^+(-\vec{p}, t)b(-\vec{p}, t)|\text{in}\rangle$$

From electroneutrality of the system follows $f^e = f^h = f$

So we obtain the basic kinetic equation of the non-Markovian type

$$\dot{f}(\vec{p}, t) = \frac{1}{2}\lambda(\vec{p}, t)\int_{t_0}^{t} dt' \lambda(\vec{p}, t')\left[1 - 2f(\vec{p}, t')\right]\cos\theta(t, t')$$

were

$$\theta(t, t') = \frac{2}{\hbar}\int_{t'}^{t} dt'' \varepsilon(\vec{p}, t'')$$

For a numerical solution, it is more convenient to represent this integro-differential equation in the form of a system of three first-order differential equations:

$$\dot{f} = \frac{1}{2}\lambda u, \quad \dot{u} = \lambda\,(1 - 2f) - \frac{2\varepsilon}{\hbar}v, \quad \dot{v} = \frac{2\varepsilon}{\hbar}u,$$

the auxiliary function $u(\vec{p}, t)$ and $v(\vec{p}, t)$ appearing here are related to the polarization effects

$$u(\vec{p}, t) = \int_{t_0}^{t} dt'\lambda(\vec{p}, t')[1 - 2f(\vec{p}, t')]\cos\theta(t, t')$$

$$v(\vec{p}, t) = \int_{t_0}^{t} dt'\lambda(\vec{p}, t')[1 - 2f(\vec{p}, t')]\sin\theta(t, t')$$

The above system of ordinary differential equations has a integral of motion

$$(1 - 2f)^2 + u^2 + v^2 = 1$$

To solve it, we must specify the initial conditions. Define the initial time as t_0 **Since the initial state is vacuum,**

$$f(t_0) = u(t_0) = v(t_0) = 0$$

We investigated different electric field dependence of the time:
constant electric field (for a given time interval)

$$E(t) = E_a = \text{const}, \quad A(t) = -E_a t$$

pulse Eckart - Sauter type

$$E(t) = E_a \cosh^{-2}(t/T), \quad A(t) = -E_a \tanh(t/T)$$

harmonic oscillations of constant amplitude with a half-integer number of cycles

$$E(t) = E_a \sin(\omega t), \quad A(t) = \frac{E_a}{\omega} - \frac{E_a}{\omega} \cos(\omega t)$$

harmonic oscillations with a Gaussian envelope

$$E(t) = E_a \cos(\omega t) \exp(-t^2/2\tau^2),$$
$$A(t) = -\sqrt{\frac{\pi}{8}} E_a \tau \exp\left(-\sigma^2/2\right) \text{erf}\left(\frac{t}{\sqrt{2}\tau} - i\frac{\sigma}{\sqrt{2}}\right) + \text{c.c.}$$

super-Gaussian pulse without filling

$$E(t) = -\dot{A}(t) = E_a \exp[-(t - t_m)^n/(2\tau^n)]$$

2. e-h excitations in graphene

**We start with the case of a constant field. The figures shows the
distribution function of carriers formed as a result of the action
of a strong constant field ~1000000 V/cm along the axes x1 in the course of ~10^-14 s**
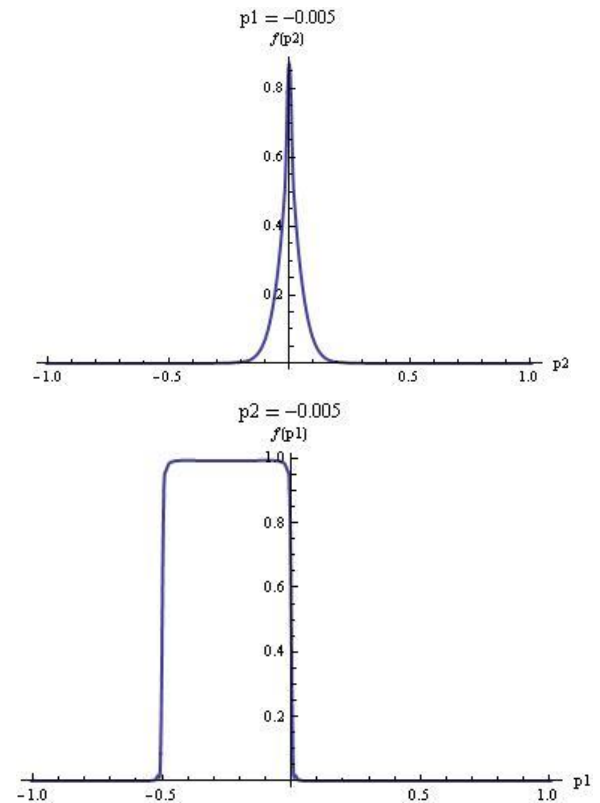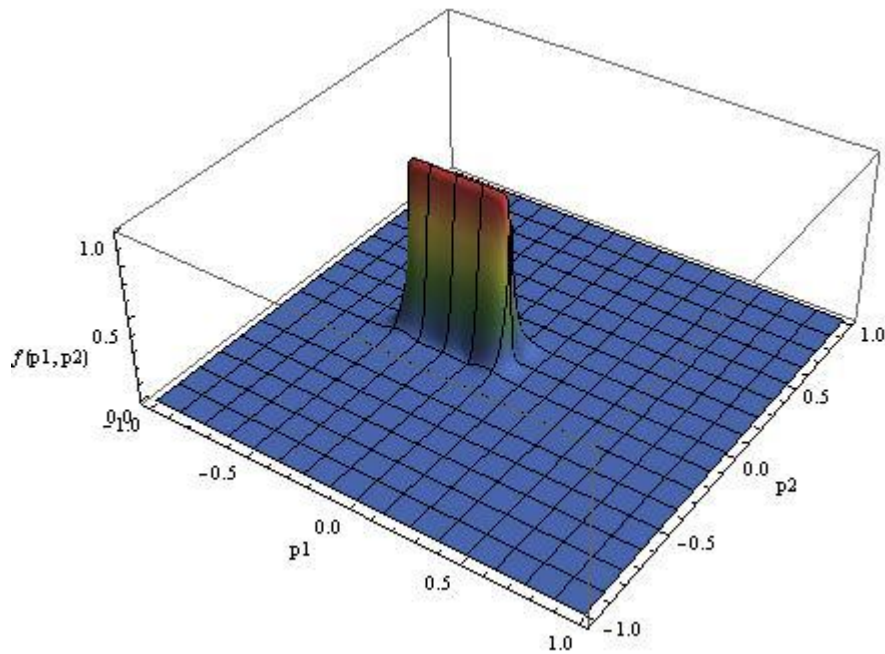
Here is the result of the action of one harmonic bipolar pulse.
The amplitude and direction of the field is the same as in the previous case.
The pulse duration is 20% of the duration of the action of the constant field in the previous case.
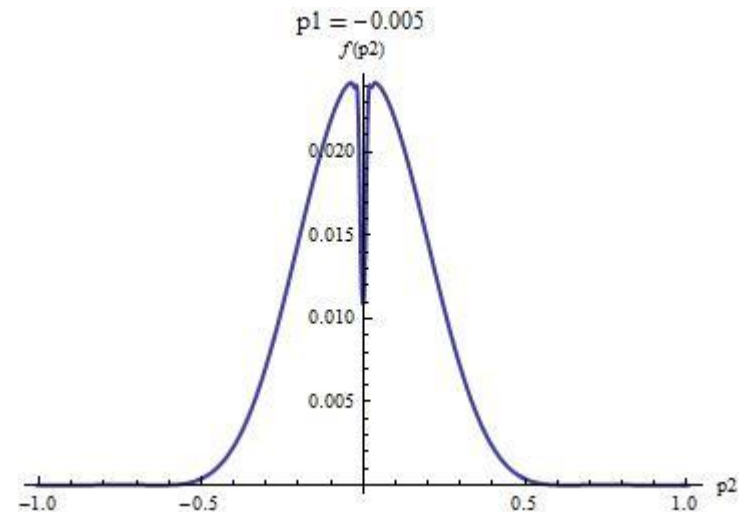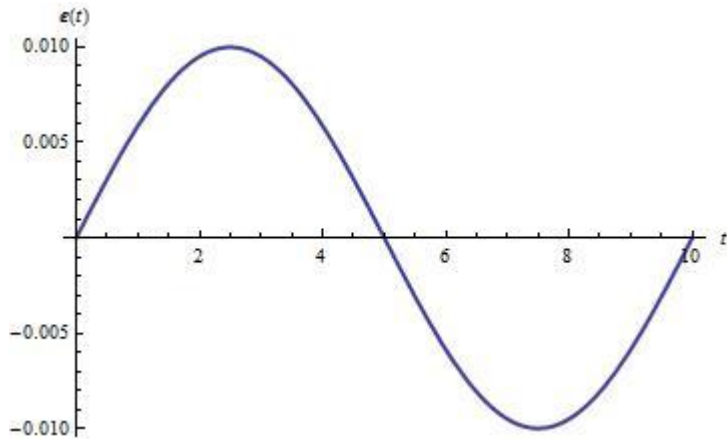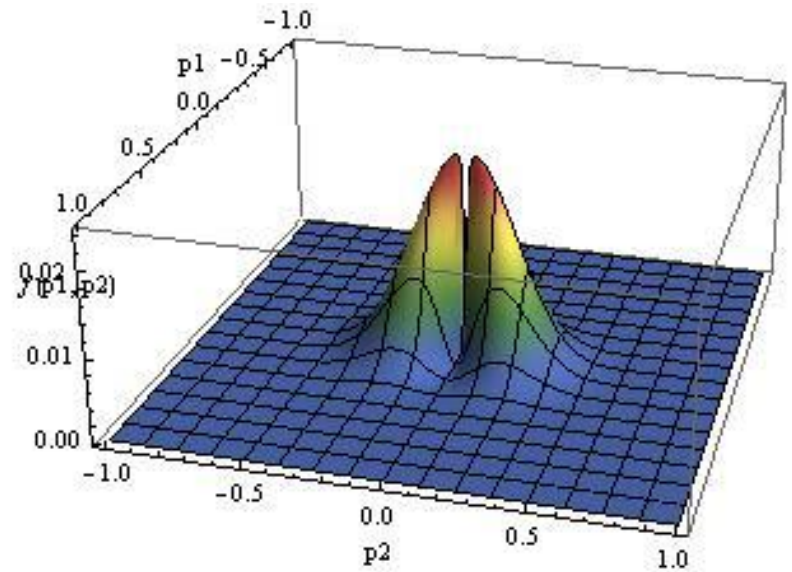
Increase the exposure time.
Now it's five full periods.
The maximum values of the
distribution function increased
approximately fifteen times.
There is a redistribution of carriers
in momentum space.
They concentrate on a circle
equidistant from the Dirac point.
But the distribution as before
anisotropic.
The direction along the active field
is preferable.
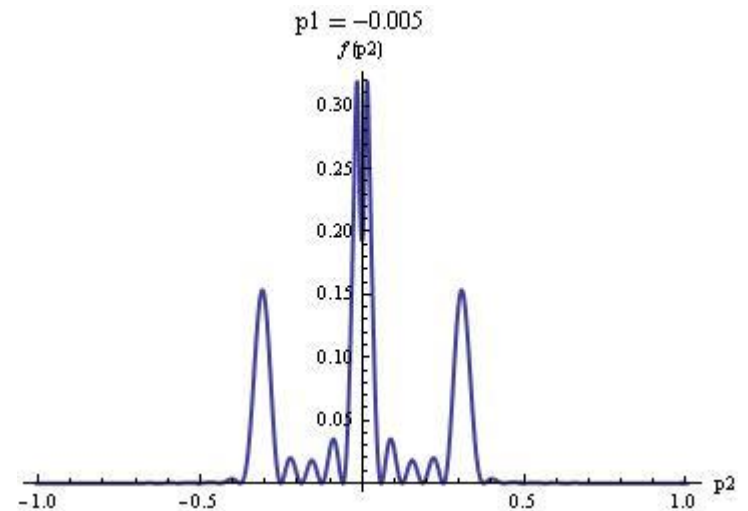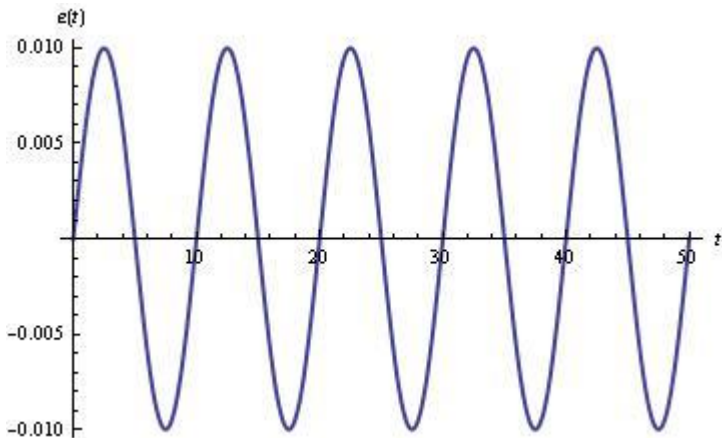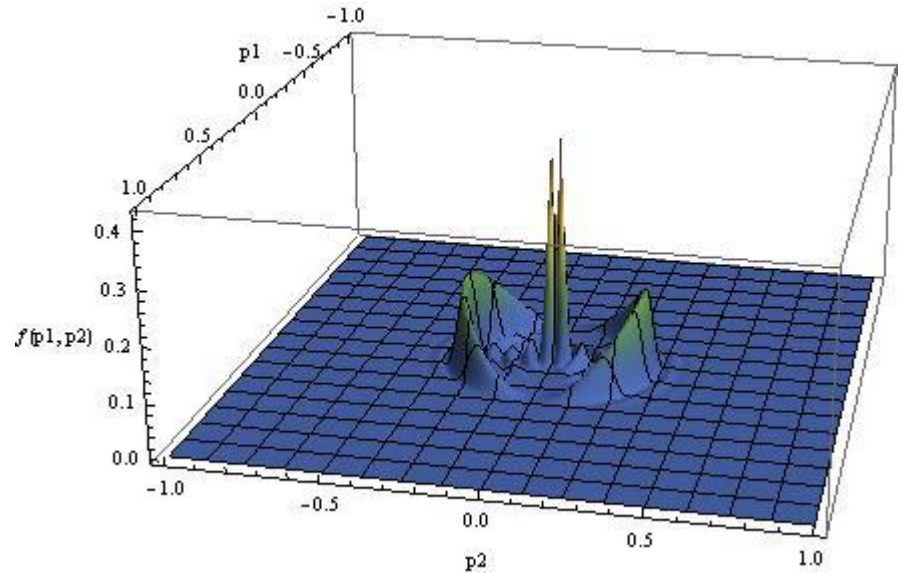
**The frequency and amplitude of the electric field oscillations have been preserved, but we will format the pulse with Gaussian cutoff symmetrically around the maximum value.
The presented dependence of the field on time and the upper 3D figure correspond to the Gaussian cutoff parameter σ = 5 ($\sigma = \omega\tau$).
For the bottom 3D figure σ = 10.**
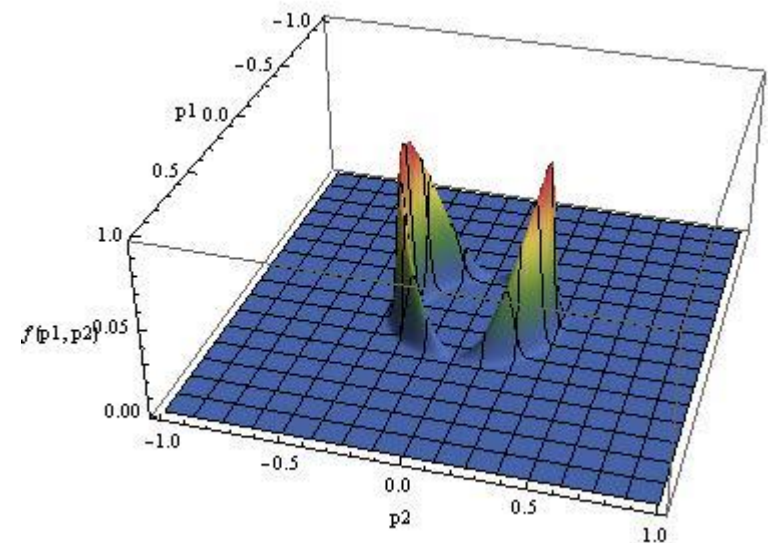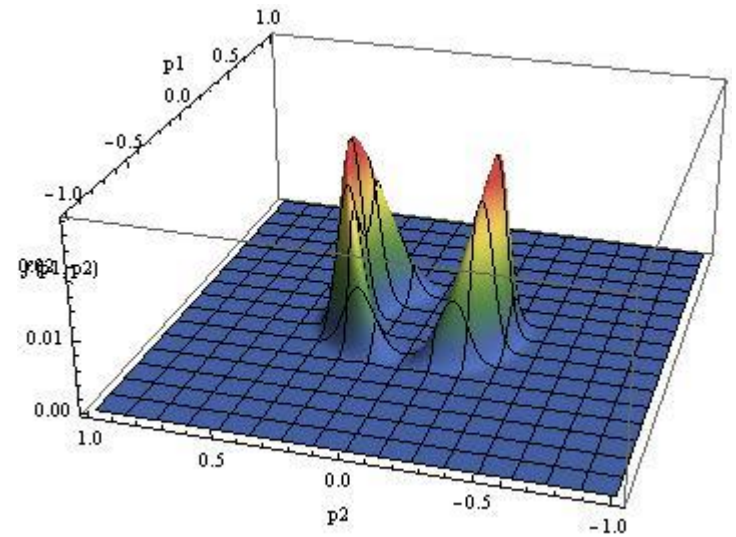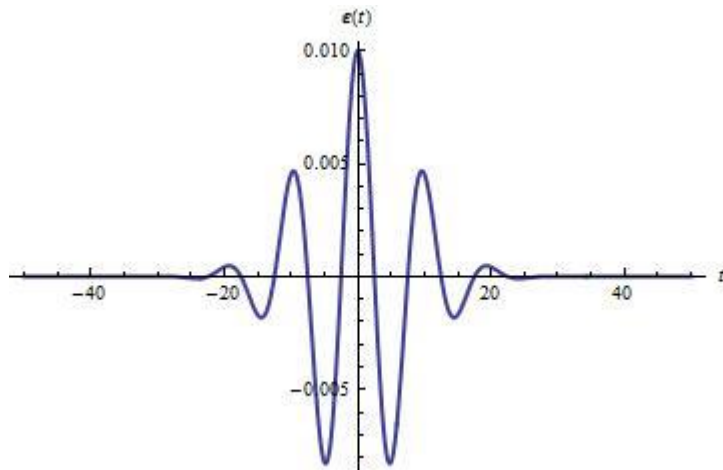
3. From linear to "circular" polarization

The above results were obtained for a constant direction of the electric field.
In the 2 + 1 dimensional model under consideration, both components of the field enter equally into KE.
This allows us not to limit ourselves to the study of fields that preserve the direction of their action.
 We can look at the result of the action of the field with changing magnitude and direction of the action.
Or consider a field of constant magnitude with a rotating direction of action.
The latter variant corresponds to a fall on a graphene layer of a circularly polarized wave.
To complete the picture, let us trace completely the transition from linear to circular polarization. To do this, we define the components of the electric field in the form:

$$
\begin{aligned}
E_x(t) &= E_a \cos(\omega t) \exp(-t^2/2\tau^2), \\
E_y(t) &= E_a \cos(\omega t - \phi) \exp(-t^2/2\tau^2)
\end{aligned}
$$

Then by changing the value of ϕ from zero to half of Pi, we can smoothly go from linear polarization to circular. Gaussian trimming is designed for a realistic model.
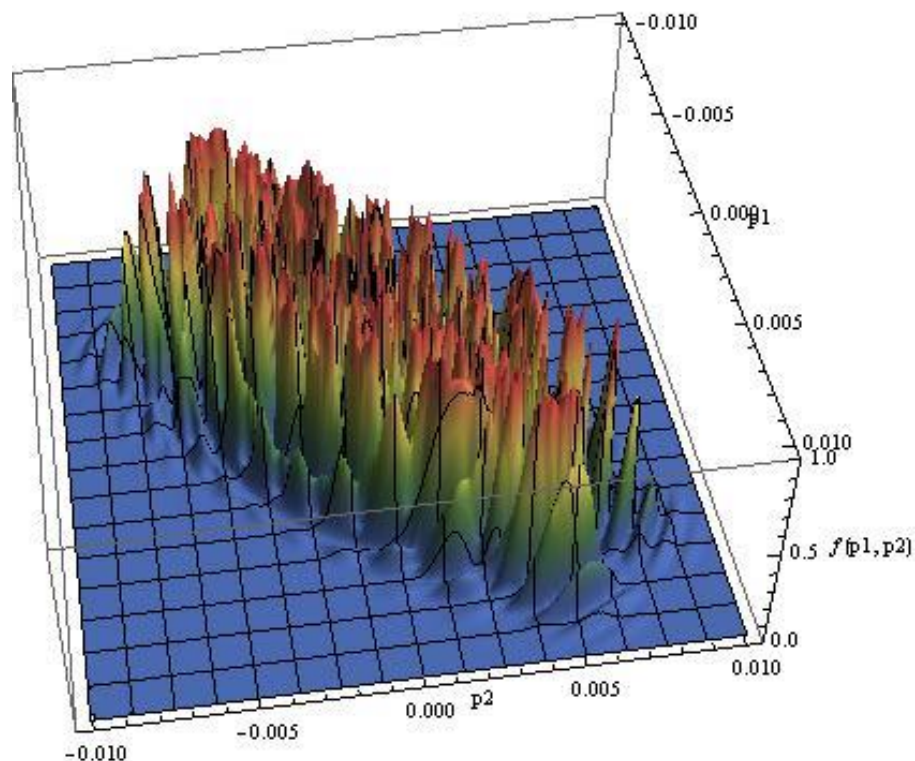
The results for the field with the following parameters are presented:

Frequency $\omega/2\pi$ = 1 THz.

The amplitude of each component 1000 V/cm.

Gaussian cutoff parameter
$\sigma = \omega\tau$ = 10.

These are quite realistic parameters.

The figure shows the form of the distribution function for ϕ = 0. This is linear polarization. The field is directed diagonally between the x and y axes and does not change its direction in time. The direction indicated by the polarization of the field is also represented in the momentum space. Although the structure of the distribution function is complex, the diagonal direction is clearly visible. We note that for the chosen pulse parameters the distribution function is concentrated in the immediate vicinity of the Dirac point. In such conditions, the applicability of the model used is undeniable.

Already at $\phi = 0.3\pi/2$

the distribution function has noticeable changes (upper figure).

The lower figure is the result of the action of a pulse with circular polarization at $\phi = \pi/2$

Another type of symmetry of the active field is reflected in the momentum space. A radial symmetry of the distribution function around the Dirac point is observed.

This symmetry is not strict. The reason is the presence of a Gaussian cutoff, which leads to a non-equivalence of the evolution of the field components in the presence of a phase shift between them.

The localization of the distribution function in the neighborhood of the Dirac point is preserved.

In all the cases considered, the maximum values of the distribution function reach saturation.
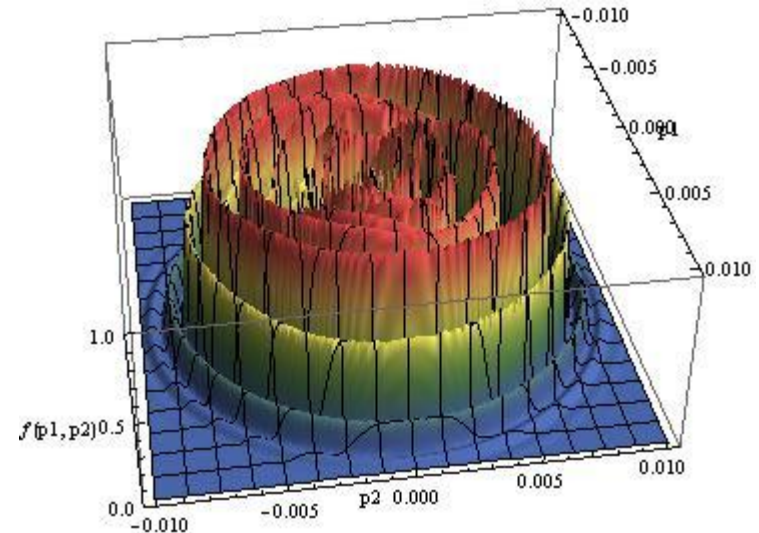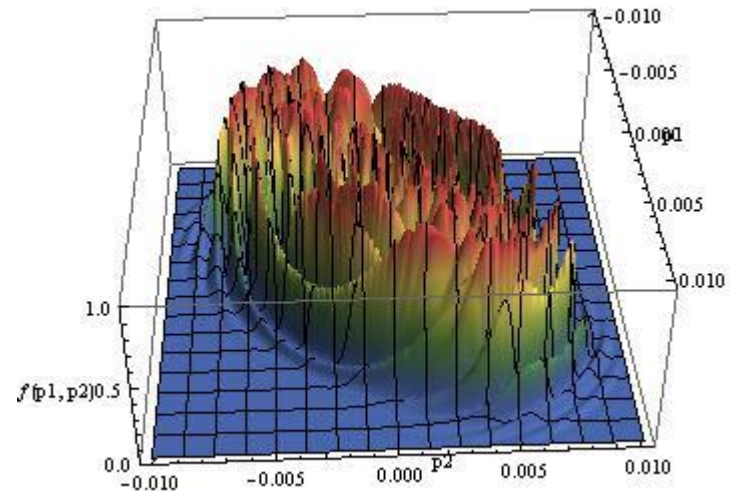
It should be noted that similar calculations are extremely difficult in the standard QED. In the case under consideration the presence of detailed information about the distribution function of carriers makes it possible to determine the observed characteristics of the model. One of the most important is the density of carriers:

$$n = \frac{4}{(2\pi\hbar)^2} \int d^2p\, f(\vec{p})$$

We present here the results of calculations of the dependence of the density of residual carriers on the phase difference between the electric field components E_x and E_y in the interval $0 \leq \phi \leq \pi/2$. The remaining parameters are the same. The transition to "circular" polarization increases the production efficiency of carriers by about 2.7 times.
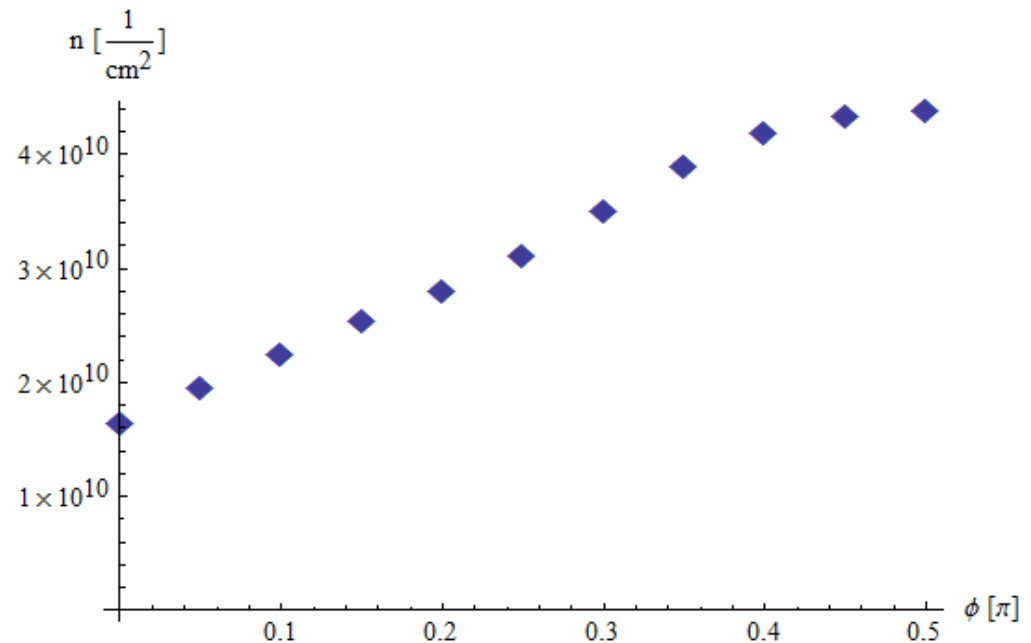
4. Residual currents

Above we showed the distribution function in the final state after the termination of an external electric field. Hence in this case we are talking about the residual density of carriers. I recall that in this model we use as the initial state a vacuum in which carriers are absent. All carriers in the final state are created during the time of the field action.

But the dynamics of the processes during the action of the field may also be of interest. First of all, this refers to currents generated by an external electric field. The currents can be related both to the motion of the created carriers and to the polarization of the physical vacuum in the external field:

$$j_i^{\text{cond}}(t) = \frac{8ev_F}{(2\pi\hbar)^2} \int d^2p \, f(\vec{p}, t) \begin{cases} v_F P_1/\varepsilon, \, i = 1 \\ v_F P_2/\varepsilon, \, i = 2 \end{cases}$$

$$j_i^{\text{pol}}(t) = \frac{8ev_F}{(2\pi\hbar)^2} \int d^2p \, u(\vec{p}, t) \begin{cases} -v_F P_2/\varepsilon, \, i = 1 \\ v_F P_1/\varepsilon, \, i = 2 \end{cases}$$

For clarity, we consider a unipolar super-Gaussian pulse.
Such a pulse should generate a certain number of charge carriers with an asymmetric distribution in momentum space. What should give some final value of the conduction current after the field is complete. Since there is no dissipation in our model (ballistic conductivity), after removal of the field, the conduction current must retain its value.
Of particular interest is the behavior of the polarization current.

Consider super-Gaussian pulse with a coefficient n = 4 and:

$$E_0 = 1.088 * 10^3 \; {}^V\!/_{cm}$$

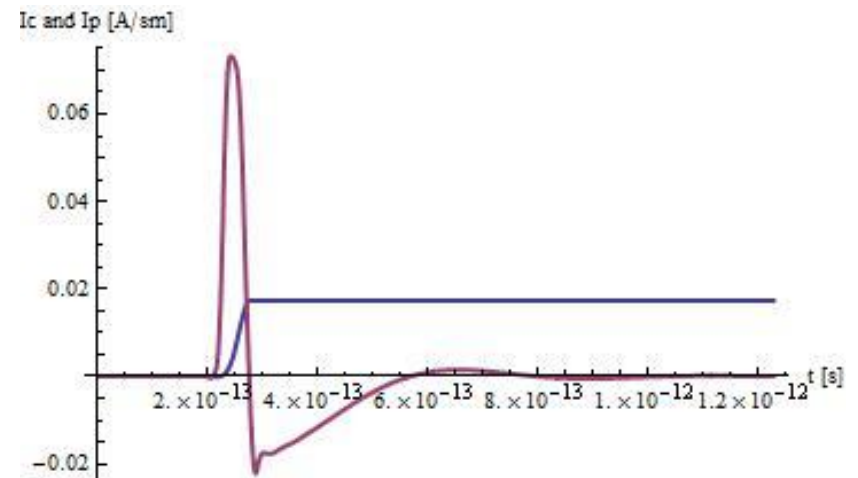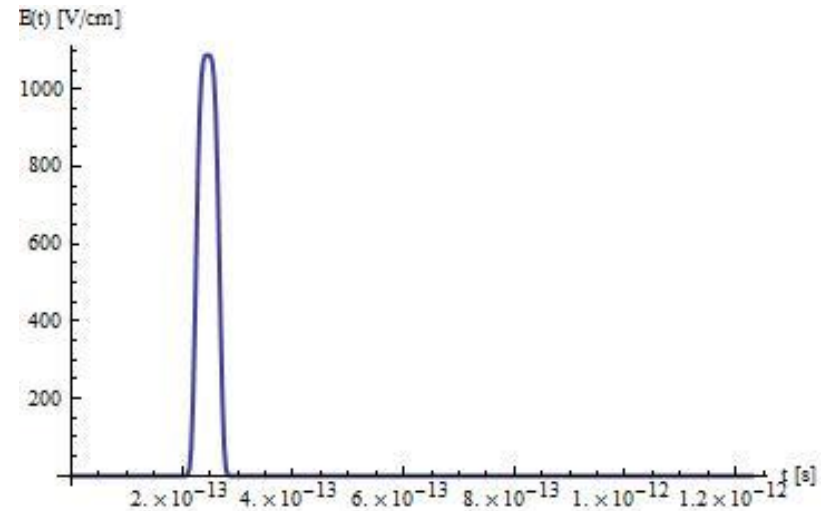$$t_m = 2.46 * 10^{-13} s$$

$$\tau = 1.23 * 10^{-13} s$$

(upper figure)

In the next figure, the blue line shows the behavior of the conduction current. It is quite expected.
The behavior of the polarization current is indicated by a purple line.
It is not so trivial.
This demonstrates the complexity of the processes of the reaction of a physical vacuum to the action of an external electric field.

5. Summary

We have obtained on nonperturbative basis the kinetic equation for describing the electron-hole excitations in graphene under the action of a spatially homogeneous electric field with an arbitrary time dependence and polarization. This is done by analogy with the well developed case o D = 3 + 1 QED kinetic theory of vacuum electron-positron plasma generation in strong fields.

The presented method makes it possible to investigate in detail the carrier generation processes, their spectrum both in the final state and during the field action.

It is possible to determine and analyze the evolution of the observed parameters for different characteristics of the active field.

The main obtained results:
- the e-h excitations are considered in different rotating field models imitating the electric fields of the elliptic polarization;
- It is showed that the "elliptic" polarized field is more effective in comparison with the linear polarized;
- it is shown that the polarization current demonstrates damping oscillation on the background constant residual conductivity current.

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THANK YOU
FOR ATTENTION