Comparison two different description of the I-V characteristic of graphene: theory and experiment

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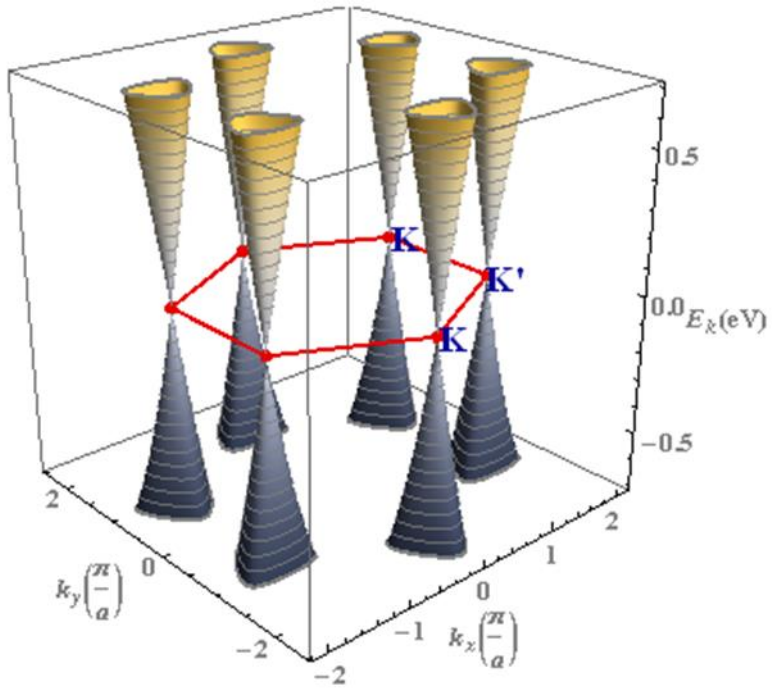

1. Introduction
2. Kinetic equation formalism
3. LDL approximation
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Introduction

At present, there is interest in a nonperturbative dynamic description of transport phenomena in condensed matter physics on the basis of methods developed for QED in the presence of strong electromagnetic fields.

For example, in the case of graphene, this is due to analogies that are found when considering this material as a quantum field system. This refers to the analogy between the process of carrier generation in this material and the creation of electron-positron pairs in strong quasiclassical electric fields (Schwinger effect).

To describe the Schwinger effect, an effective approach was developed based on the quantum kinetic equation (KE) [S. Schmidt, D. Blaschke, G. Röpke, S.A. Smolyansky, A.V. Prozorkevich and A.D. Toneev Int. J. Mod. Phys. E v. 7, 709 (1998)]. It has proved itself well and allows modeling processes with an arbitrary dependence of the effective field on time [D.B. Blaschke, B. Kampfer, S.M. Schmidt, A.D. Panferov, A.V. Prozorkevich and S. A. Smolyansky, Phys. Rev. D v. 88, 045017 (2013)].

The version of the method for graphene was realized taking into account its 2D structures and the specific law of dispersion of carriers. Like any new approach, the proposed approach needs to be verified by comparison with other theoretical methods and experimental results.

The purpose of the proposed report is to check the correctness and effectiveness of the developed formalism. As a test, the standard problem of calculating the I-V characteristic for a graphene sample was chosen. We want to show that in the case of a ballistic non dissipative regime, a new approach leads to the same results as the Landauer-Datta-Lundstrom (LDL) approach:

N. Vandecasteele, A. Barreiro, M. Lazzeri, A. Bachtold and F. Mauri, Phys. Rev. B82, 045416 (2010),

B. Dora and R. Moessner, Phys. Rev. B81, 165431 (2010),

G. Kané, M. Lazzeri and F. Mauri, J. Phys.: Condens. Matter 27, 164205 (2015).

In LDL approach the interaction of carriers with electric field is described in terms of the spatial dependence of their potential energy (x - representation). For the constant electric field we have the expression $eV(x) = -eEx$.

The presented KE formalism uses an alternative method of describing the interaction with a field through the introduction of a quasimomentum $P = p - \frac{e}{c}A(t)$.

The characteristic of the field in this case is the vector potential $A(t)$. This function in the presence of a field is necessarily time dependent. In the simplest case of a constant electric field it is linear in time $A(t) = -Et + C$, where C is an arbitrary constant. Therefore, we will refer to this approach as a t - representation.

It is assumed that both approaches should lead to the same physical characteristics of the described process.

The represented t-approach based on the kinetic equation is not the only possible one. Note the article:

S.P. Gavrilov, D.M. Gitman and N. Yokomizo, Phys. Rev. D86, 125022 (2012)

in which the behavior of the exact solutions of the Dirac equation in the presence of a constant electric field in the two-dimensional case is studied in detail. Including graphene. Although only qualitative estimates are presented, they are in good agreement with the results of other approaches.

2. Kinetic equation formalism

The starting point is the Dirac-type equation for low-energy excitations in graphene in the presence of the electric field

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

where $\hat{P}_k=-i\hbar\nabla_k-(e/c)A_k(t)$ **is the quasi-momentum** $(k=1,2)$, σ_k **are the Pauli matrices corresponding to the pseudospin structure of graphene.**

For the physical interpretation of the model it is appropriate to go over to the quasiparticle representation, where the Hamiltonian of the theory is diagonal. It is reached with help of the unitary transformation

$$U^{\dagger}(t)v_F\vec{P}\vec{\sigma}U(t)=\varepsilon(\vec{p},t)\sigma_3=H_{\vec{p}}(t),$$

and $\Phi=U^{\dagger}\Psi$ **with the unitary matrix**

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

The function $\varkappa=P^2/P^1$

The quasienergy determined by the dispersion relation in the vicinity of the Dirac points:

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

Final integral form of the kinetics equation of non-Markovian type is universal:

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

where

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

The features of the behavior of the system are determined by the dispersion law and by the expression for the transition probability:

$$\lambda(\vec{p},t) = \varkappa = \frac{ev_F^2[E_1P_2 - E_2P_1]}{\varepsilon^2(\vec{p},t)}. \qquad (3)$$

This KE is written for zero initial condition, $f(t_0) = 0.$

The main feature consider KE for graphene is the absence of an energy gap in the quasienergy.

For the numerical analysis of the KE for different field models it is appropriate to rewrite it in the form of an equivalent system of ordinary differential equations

$$\dot{f} = \frac{1}{2}\lambda u, \quad \dot{u} = \lambda(1-2f) - \frac{2\varepsilon}{\hbar}v, \quad \dot{v} = \frac{2\varepsilon}{\hbar}u, \qquad (4)$$

with the corresponding initial conditions $f(t_0) = u(t_0) = v(t_0) = 0.$

For this system of equations one readily obtains the integral of motion

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

which is compatible with the initial conditions.

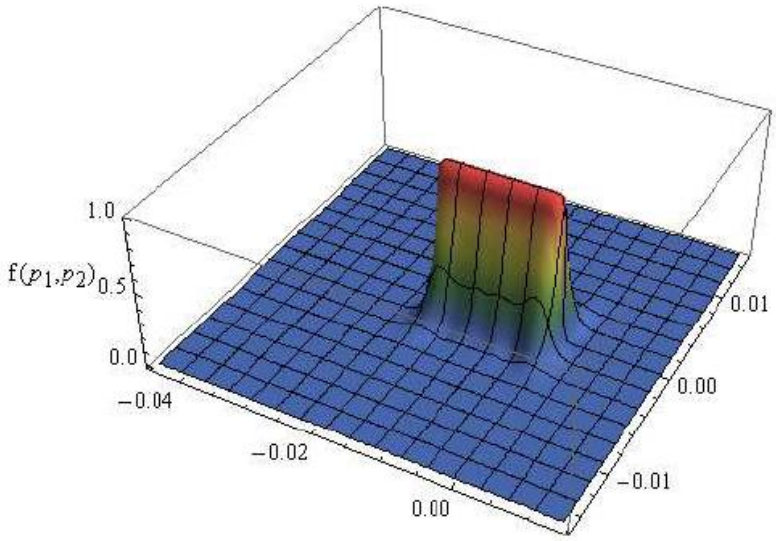
Since our main goal is to compare the predictions about the I-V characteristics of graphene samples with a constant potential difference, we consider in detail the case of a constant field of the form:

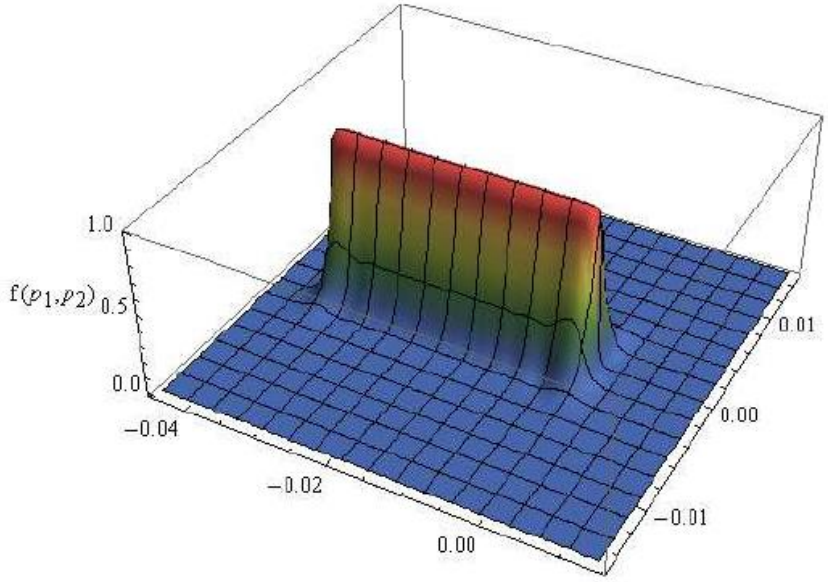
$$E_1(t) = E_0 = \text{const}, \quad A_1(t) = -E_0 t, \qquad E_2(t) = 0, \quad A_2(t) = 0, \tag{5}$$

for the case when the coordinate system is oriented taking into account the direction of the field action.

Having at our disposal the KE (2) (or (4)), we can obtain complete information about the characteristics of the carriers for any time.

The figure shows the form of the distribution function in the vicinity of the Dirac point for two instants of time $t = 0.5 \times 10^{-12}$ and $t = 1.0 \times 10^{-12}$ s. The distributions presented are the result of the action of the electric field $0.1\ V/\mu m$ on the initial vacuum state.





We observe the process of carriers generation. The rate of their generation is constant in time.

The next necessary step is the transition to integral characteristics of the distribution function.
As such we can consider the carrier density

$$n(t) \;=\; 8\int [dp] f(\vec{p},t), \tag{6}$$

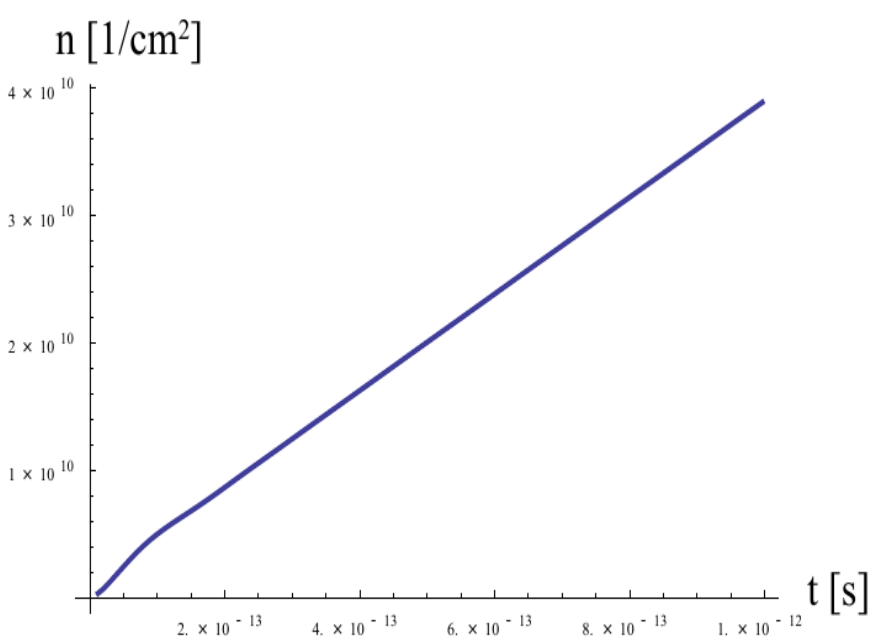
and the density of the conduction current

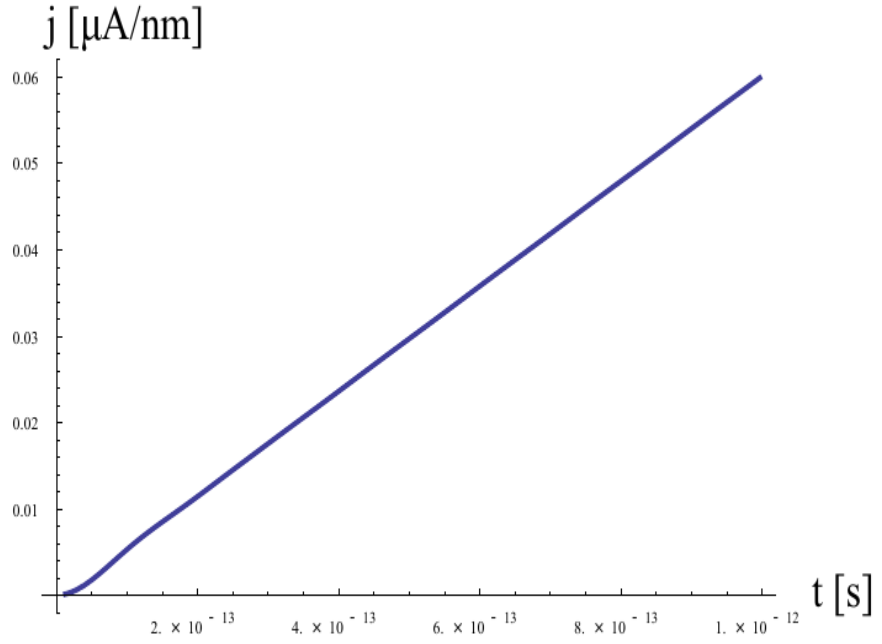
$$j_i^{\mathrm{cond}}(t) \;=\; 8ev_F^2 \int [dp] f(\vec{p},t)\frac{P_i}{\varepsilon(\vec{p},t)}, \tag{7}$$

Here the abbreviation $[dp] = d^2p(2\pi\hbar)^{-2}$ has been used.
The coefficient 8 takes into account two-valley degeneracy, two variants of the quasispin value and the equivalence of the contribution of quasielectrons and holes.

Since the problem is two-dimensional, these are surface densities.
Formalism assumes spatial homogeneity of the system, hence these integral characteristics will depend only on time

The dependence of charge carrier density (6) and conductivity current density (7) on time for the field (5) is shown on this slide.
The two charts presented are remarkably similar, which, incidentally, can not be considered a surprise. They clearly reflect the linear nature of the accumulation of carriers in the non dissipative regime and, correspondingly, a linear increase of the current:



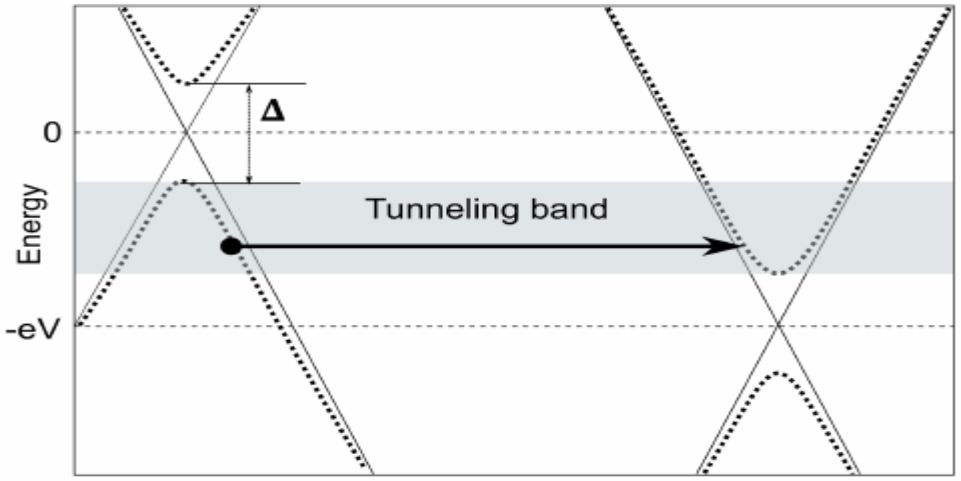


3. LDL approximation

In the Landauer-Datta-Lundstrom (LDL) approach, the problem of calculating the current density through the sample of a material of finite width is solved by calculating the tunneling probability in the presence of a given potential difference V [N. Vandecasteele, A. Barreiro, M. Lazzeri, A. Bachtold and F. Mauri Phys. Rev. B82, 045416 (2010)].

$$j_{LDL} = \frac{4e}{(2\pi\hbar)^2} \int dp_2 \int_{\varepsilon_F - eV}^{\varepsilon_F} d\varepsilon \; T(\varepsilon, p_2, V), \tag{8}$$

where $T(\varepsilon, p_2, V)$ is the probability that an electron is transmitted through the sample.
As before field is directed along the first axis of coordinates. Therefore, the momentum component p_2 does not change its value during tunneling.
In spite of the fact that graphene is a gapless semiconductor, the presence of finite conserved values p_2 leads to the appearance of an energy gap with the width $\Delta = 2v_F p_2$:



The process of passing carriers through it has the character of quantum tunneling.
The probability of such a tunneling in the WKB approximation for the distance L between the electrodes :

$$T(\varepsilon, p_2, V) = \exp[-\frac{\pi p_2^2 v_F L}{e\hbar V}]. \quad (9)$$

For pure tunneling, integrating (8) using expression (9), one can obtained

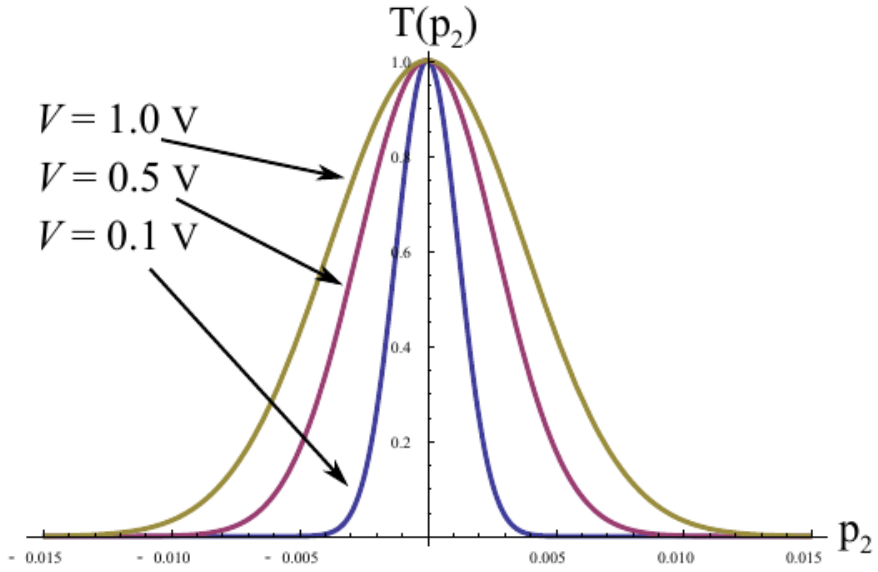
$$j_t = 2\frac{Ve^2}{\pi^3 \hbar L}\sqrt{\frac{\pi^2 eVL}{4\hbar v_F}} \times \left(\mathrm{erf}\left[\sqrt{\frac{\pi eVL}{4\hbar v_F}}\right] + \exp\left[-\frac{\pi eVL}{4\hbar v_F}\right] - 1\right). \quad (10)$$

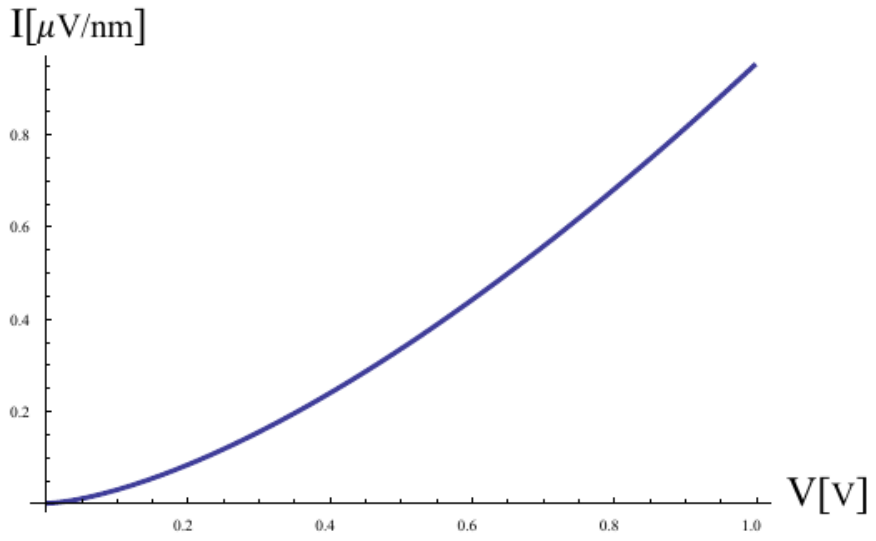
The results of the theory for this case are shown in figure.

The left panel shows the dependence of the tunneling probability on the transverse momentum for three values of the potential difference V.

First of all, it should be noted that for any, even the smallest, potential difference at small transverse momenta (in the vicinity of the Dirac point), the probability of a transition from electrode to electrode is close to unity. This is a natural consequence of the contact between the valence band and the conduction band at this point. We also note that the tunneling probability decreases sharply $T(p_2) \sim exp\{-Cp_2{}^2\}$ with increasing momentum p_2 which is a direct consequence of the expression (9).

The width of the tunneling region increases with increasing electric potential difference V. This leads to an increase in the integral tunneling current density I through the sample (right panel).





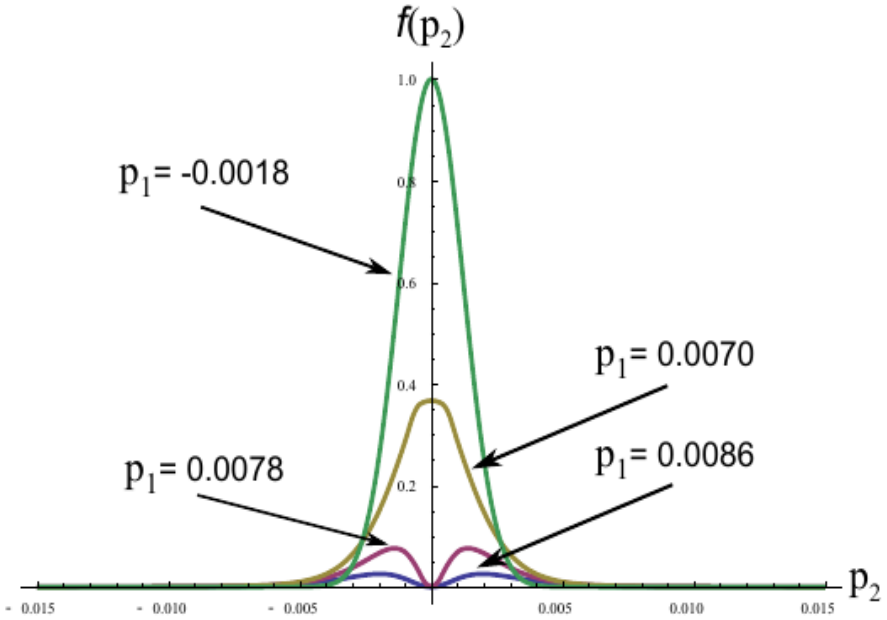
4. Comparison of the two approaches

What is common in the presented results?

From the point of view of model LDL, the current through the sample is provided by a carrier flow having a well-defined transverse momentum distribution (figure on the previous slide).

And what is the distribution over the transverse momentum of carriers generated by a constant field according to the kinetic approach? The shape of the cross section $f(p_2)$ of the distribution function is formed at the initial stage of the process and is then reproduced in an unchanged form at ever larger values of the p_1. This process is shown in the next figure.

At $p_1 \approx 0.0$ the profile of the section is formed finally and then remains unchanged. The figure shows this constant profile shape for $p_1 = -0.0018$.

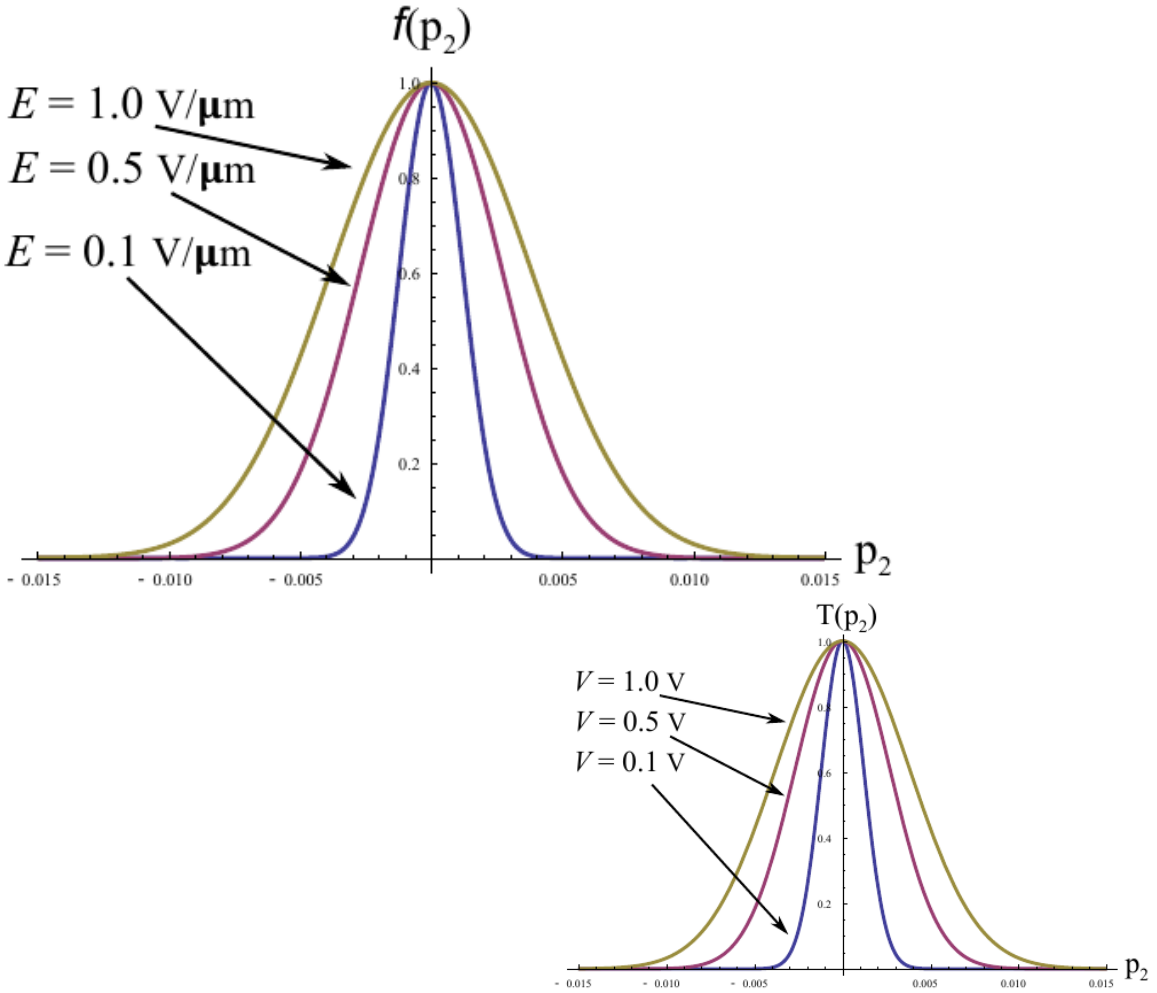


With the exception of the initial and final sections of the distribution function, it is this profile that determines the contribution of carriers with different values p_2 to the current density generated by the field.

The shape of the $f(p_2)$ changes when the strength E of the active electric field changes. Figure shows the form of this function for three values of the field strength. The values of the electric field strengths are equal to those that arise in a sample with length $L = 1.0\,\mu m$ when a potential difference $V = 0.1, 0.5, 1.0\,V$.

Comparison of the $f(p_2)$ with $\mathrm{T}(p_2)$ shows their coincidence. It demonstrates that both approaches predict the same p_2 dependence of the carrier distribution function and the same behavior of this dependence of the electric field strength in the sample.

The advantage of the t-re presentation is the possibility to obtain complete and arbitrarily detailed information about the distribution function.



It is possible to speak about the correctness of the predictions of the t - representation only if we can obtain within its framework the correct form of the I-V characteristic for a graphene sample of finite size. Because it is the most accessible for experimental verification.

On the way to this there is an obvious problem. It consists in the contradiction between the assumption of the spatial homogeneity of the physical vacuum considered in the t - representation and the finite size of the real sample.

As the first step to resolve this contradiction, we note that our definition of the characteristics of the system (dispersion law) is obtained by taking into account the interaction of only the nearest neighbors with a lattice constant $a = 0.246\ nm$ [P.R. Wallace, Phys. Rev. 71, p. 622-634 (1947)].

Consequently, on scales $L \gg 1.0\ nm$, the behavior of carriers should not differ significantly from the behavior in the absence of spatial boundaries. Since real experiments are performed on samples with $L \approx 1000\ nm$, this condition is guaranteed to be fulfilled.

Nevertheless, if we look at the picture presented earlier, we see that the current density in the absence of spatial boundaries under the action of a constant field increases continuously. Which, obviously, is not observed in the experiment, where each value of the potential difference corresponds to its steady-state current density. Why and how is this constant value formed?

If our assumption that the process of carrier generation is described correctly by the kinetic equation, then the cause should be sought in the interaction of the system with the electrodes:

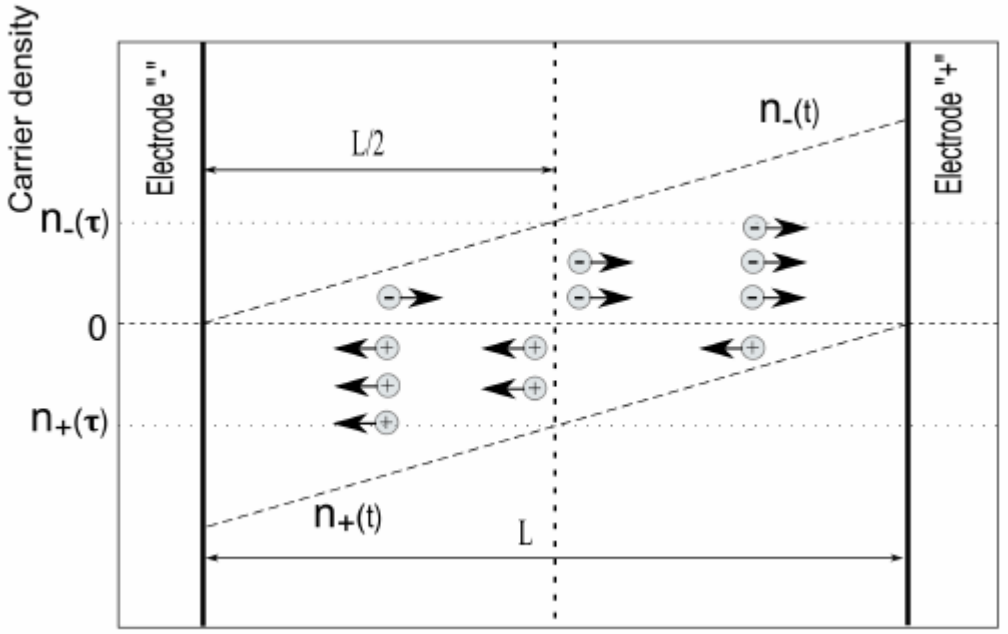
The field is present only in the interelectrode space.

It is homogeneous.

Consequently, the process of carrier generation must permanently continue throughout the entire measurement process and be uniform in the area of the sample.

But the lifetime of these carriers is not great.
Knowing the strong anisotropy of the carrier distribution function, it is possible to assume in the first approximation that all of them move toward the electrode of the corresponding polarity with a velocity v_F. In this case, the field action time is limited by the value $\tau = L/v_F$.

We will proceed from the fact that after the field is turned on, in the interelectrode space the process of carrier generation starts and continues at a constant speed as long as the field acts. Simultaneously the process of the carrier outflow through the electrodes act. The outflow is compared with the rate of their generation.
The established current corresponds to that which would have been achieved in the absence of boundaries in time τ.
These are very short time interval.



A comparison of the resulting values for j in x- and t - representation is given in table.

The results are very close.

$V\ [V/\mu m]$	j in x - representation $[\mu A/nm]$	j in t - representation $[\mu A/nm]$
0.1	0.02904	0.02964
0.2	0.08344	0.08457
0.3	0.15435	0.15557
0.4	0.23861	0.24003
0.5	0.33440	0.33601
0.6	0.44048	0.44194
0.7	0.55595	0.55725
0.8	0.68011	0.68137
0.9	0.81239	0.81335
1.0	0.95233	0.95297

Each value presented for the t - representation is the result of numerical integration on adaptable mesh of about 300 x 150 points in momentum space. To calculate the values of the distribution function at each of these points, it is necessary to solve the system of equations (4) independently.

Such a path is fundamentally more difficult than the use of expression (10).

In the case under consideration, it was done in order to demonstrate the rigorous reproduction of the results of the already approved approach. But this difficult path can be a valid alternative outside the framework of the applicability of the x - representation.

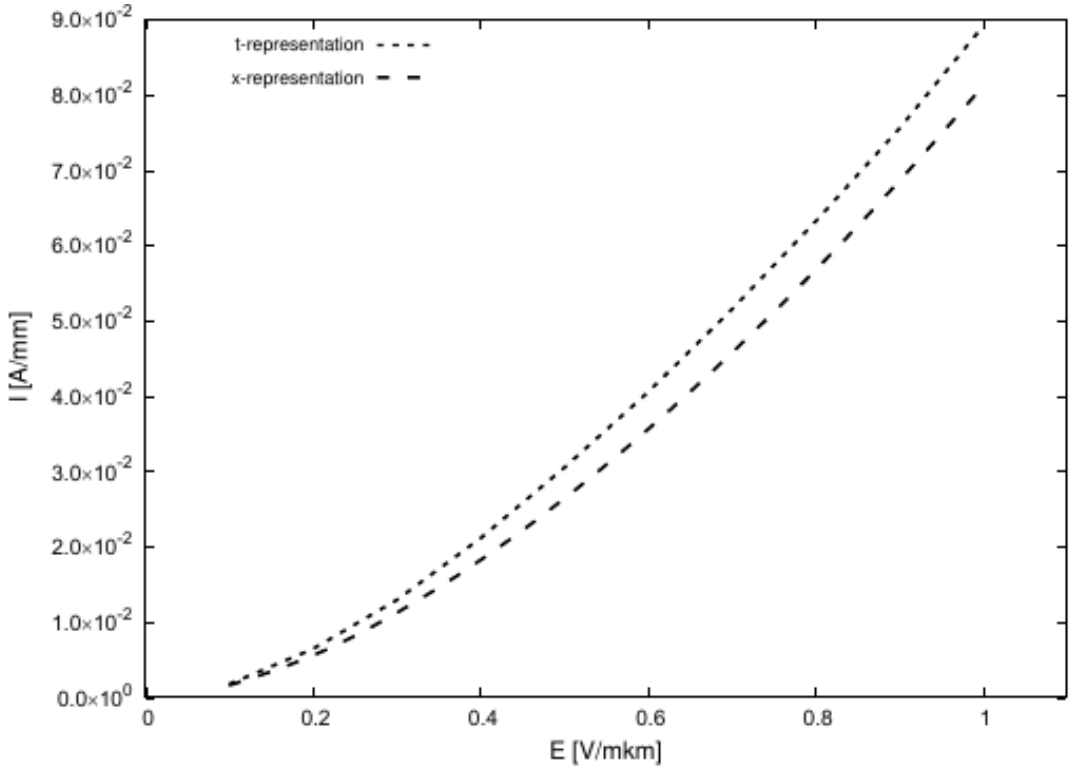
Accurate reproduction of the results of the LDL approximation for a particular experimental configuration allows one to speak of the correspondence with the experimental results in the chosen range of parameters.

KE approach can be a valid alternative outside the framework of the applicability of the x - representation. For example, in alternating electric fields in the region of sufficiently high frequencies.

A qualitative confirmation of this assumption can be obtained by estimating the previously introduced parameter τ as the characteristic time of the process. Then there is reason to believe that for samples with a smaller inter-electrode distance, the predicted values of the ballistic current will not be so coincident. To test this hypothesis, calculations were made of the ballistic current in the same range of field strengths for a sample with an inter-electrode distance of 100 nm.

The results are shown in the figure.

Already in this case, the difference for results reaches almost 10% and can be subject to experimental measurement.



5. Conclusion

1. The report presents a kinetic theory that allows one to describe carrier generation processes and the evolution of their distribution function in graphene under the action of an external electric field.

2. The possibilities of this method for a constant electric field with realistic parameters and vacuum initial state are demonstrated.

3. It is shown that the process parameters calculated in the kinetic approach are in accordance with the predictions of the LDL approximation, which is a recognized and verified method for estimating the parameter during experiments with graphene samples.

4. A key advantage of the kinetic approach is the ability to investigate the response not only to a constant electric field, but also to an electric field with an arbitrary time dependence.

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THANK YOU
FOR ATTENTION

In the presented figure, we actually observe the process of carrier generation. The rate of their generation is constant in time.

The distribution of the populated states is strictly correlated with the direction of the field action.

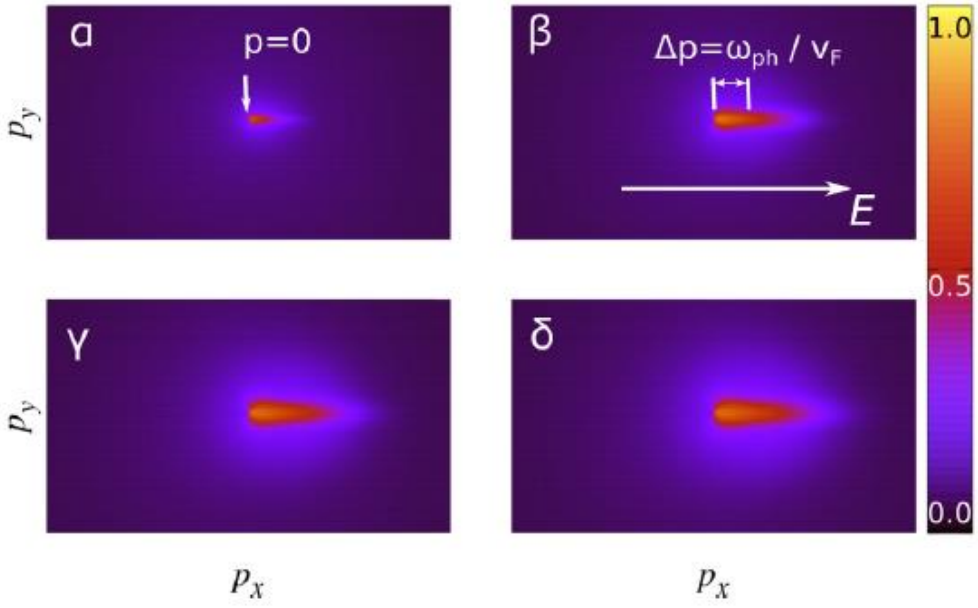
The width of the populated region in the direction perpendicular to the action of the field is constant and at the level 0.5 of the maximum of the distribution function is only 0.003 ħ/a.

While within the considered time 1.0x10^-12 s, the range of occupied states in the ``field'' direction reaches almost 0.04 ħ/a. The distribution is anisotropic and nonequilibrium.

The population of previously occupied states does not change, which reflects the absence of dissipation in the model under consideration.

With the passage of time, states are populated with ever larger values of the p_1 and, consequently, of energy. [This is in agreement with the results F. Fillion-Gourdeau and S. MacLean, Phys. Rev. B92, 035401 (2015)].

The presented data on the distribution function are in conformity with the results obtained for a constant electric field using the nonequilibrium Green's-function technique [J. Li, J.E. Han Phys. Rev. B97, 205412 (2018)] (taking into account the differences brought about by inclusion in the latter case the inelastic scattering processes provided by optical phonons).

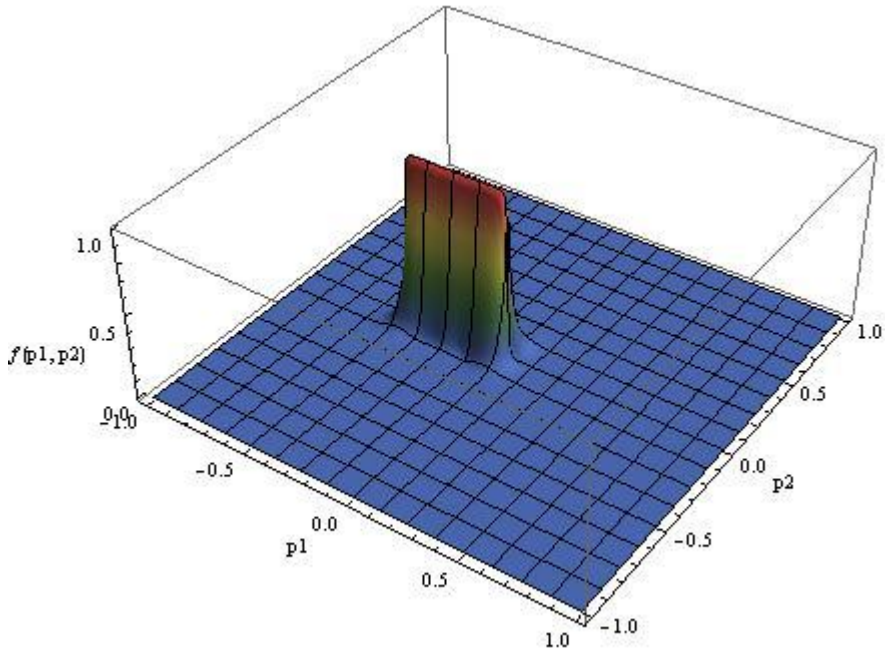


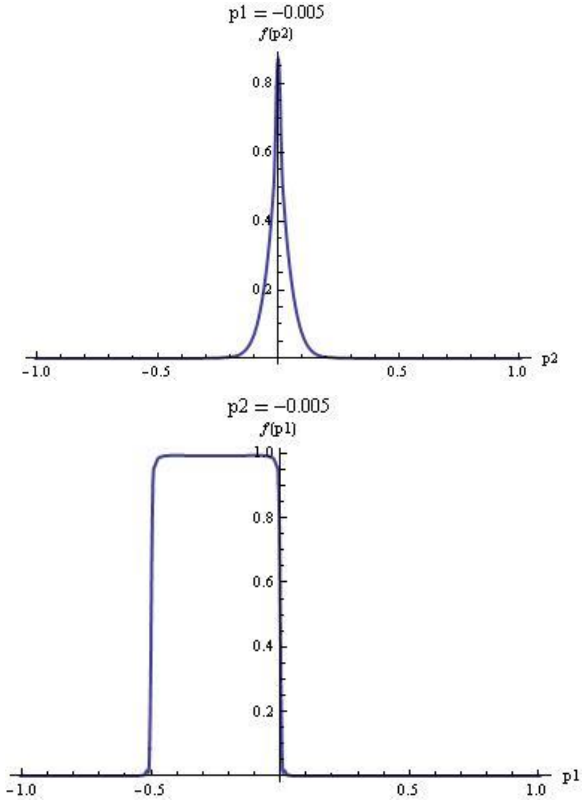
Summarizing the impression from the figure, we can say that all the appearing carrier move practically parallel along the direction of the action of the field and, by virtue of the dispersion law (1), with the same group velocity close to v_F.

In addition, we note that the results obtained confirm the correctness of using the dispersion law in the form (1). Strictly speaking, the expression (1) is valid only in the vicinity of the Dirac points. Since the total area of the Brillouin zone is $2\pi \times 2\pi$ ħ/a, it is obvious that the region of momentum space represented in the figure is the nearest neighborhood of one of them.

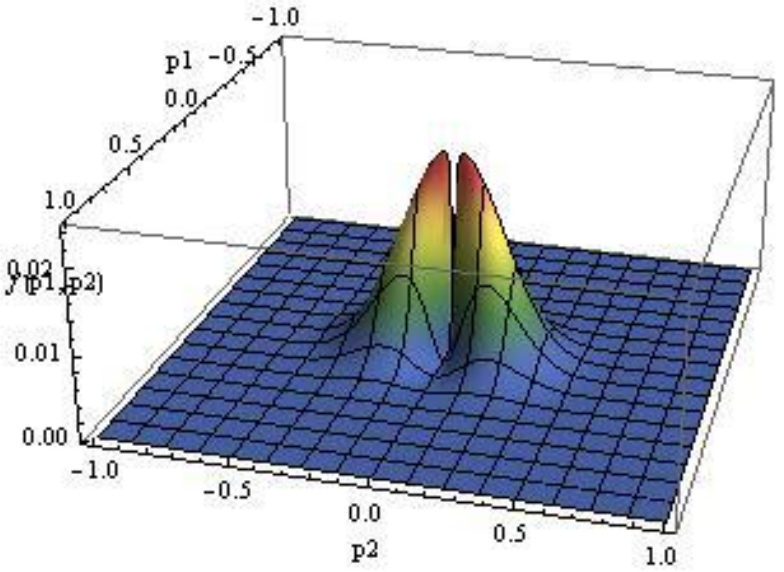
5. Numerical results
5.1 Distribution unction

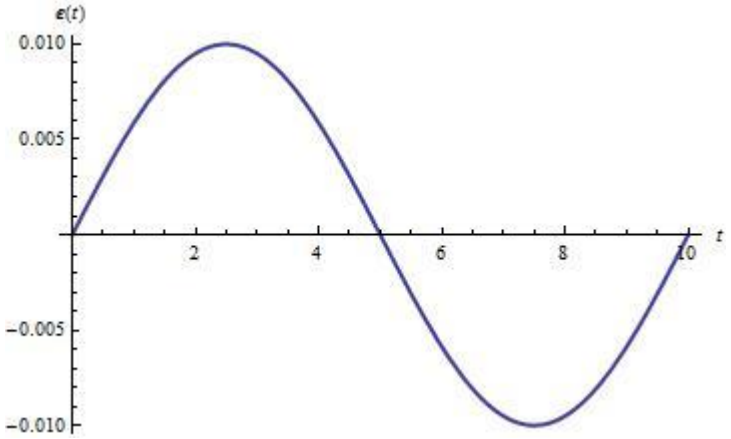
We start with the case of a constant field. The figures shows the distribution function of carriers formed as a result of the action of a strong constant field ~1000000 V/cm along the axes x1 in the course of ~10^-14 s

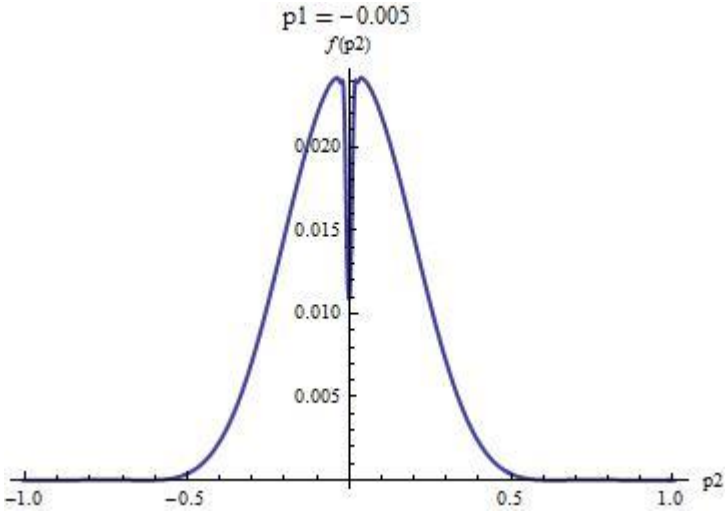




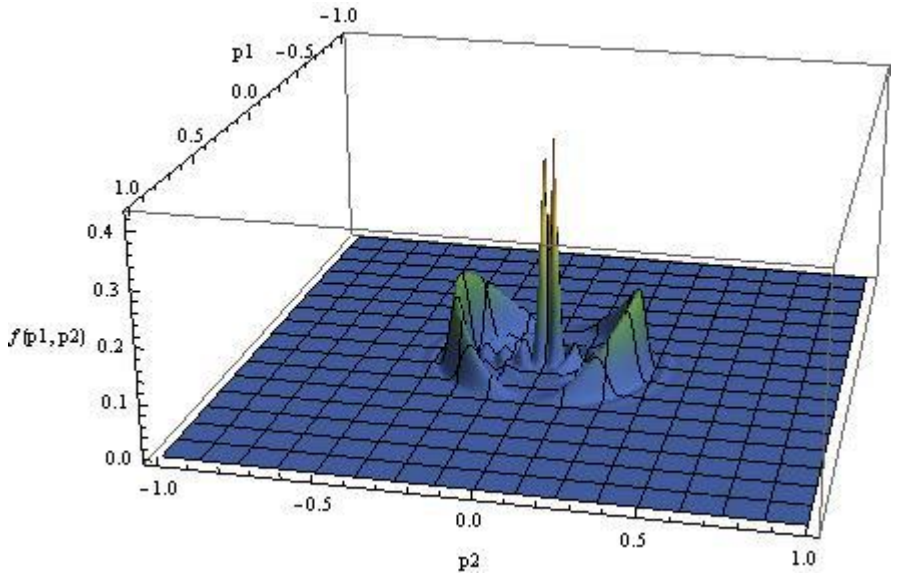
Here is the result of the action of one harmonic bipolar pulse.
The amplitude and direction of the field is the same as in the previous case.
The pulse duration is 20% of the duration of the action of the constant field in the previous case.

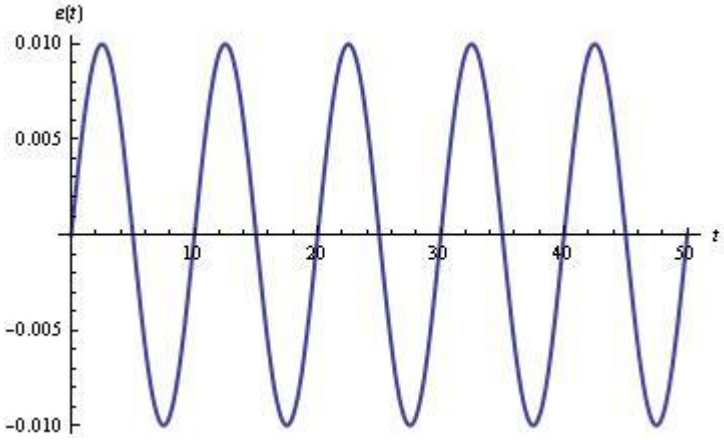


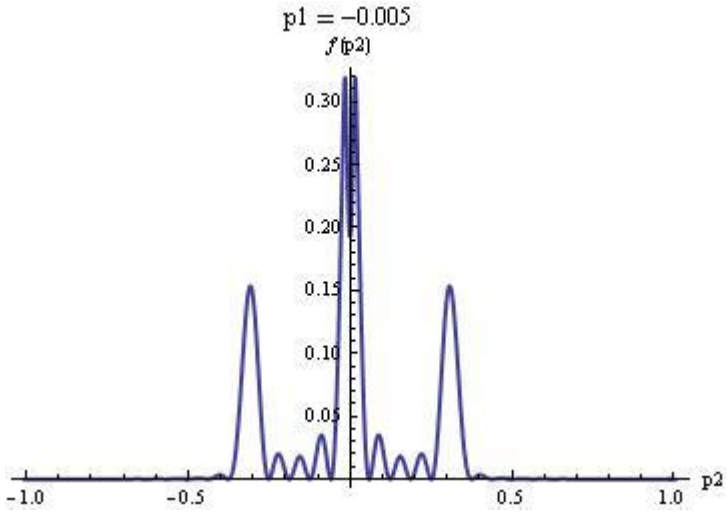




Increase the exposure time.
Now it's five full periods.
The maximum values of the distribution function increased approximately fifteen times.
There is a redistribution of carriers in momentum space.
They concentrate on a circle equidistant from the Dirac point.
But the distribution as before anisotropic.
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.