

Three-dimensional Extremely Short Optical Pulses in Graphene with Inhomogeneities

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We consider the Maxwell's equations for an electromagnetic field, which propagates in impurity graphene with taking into account the spatial inhomogeneity. By heterogeneity, we mean the presence of a region of increased electron density. A particularly important case is inhomogeneity due to areas of increased concentration of conduction electrons due to the presence of impurities. According to this fact, it seems appropriate to investigate the impact of such inhomogeneity on the pulse propagation in impurity graphene. Due to the diversity of impurities and the nature of their interaction with the graphene subsystem, different approaches are possible in such problems. One of these approaches is to consider the scattering of ballistic electrons in graphene by impurities. Impurities are considered responsible for the occurrence of a disorder and a weak localization. In this case, they go beyond the limits of the self-consistent Born's approximation and the renormalization-group approach is applied. In this paper, the electronic spectrum for the graphene subsystem is taken from the approach of the renormalization group, widely used in quantum field theory, when the transition from areas with lower energy to areas with more energy is caused by a change in the scale of consideration of the system. The main idea is that the Fermi velocity is renormalized, which begins to depend on the electron energy in a logarithmic way. Within the framework of the semi-classical approach, an effective equation for the vector-potential of the electromagnetic field is obtained and solved numerically. It is observed that three-dimensional extremely short optical pulses propagate unstably with disturbed pulse shape. In this case, the introduction of a spatial inhomogeneity of the charge density into the medium makes it possible to reduce the pulse loss in the amplitude. The influence of the spatial parameters of the inhomogeneity on the propagation pattern of an extremely short optical pulse is also studied. It is shown that the depth and the width of the spatial inhomogeneity of the charge density do not have a significant impact on the pulse shape.

Keywords: Ultrashort pulse, Graphene, Inhomogeneity, Charge density.

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1. INTRODUCTION

Recently, the propagation of extremely short optical pulses in various nano-objects has attracted the attention of researchers [1-5]. This is due primarily to the prospects for the use of such pulses for solving various kinds of problems of modern nanoelectronics. An extremely short pulse is called a pulse consisting of several oscillations of an electric field with a duration of several femtoseconds in the optical range. In this work, the semi-classical approach is used, when light is viewed from the point of view of a classical object, and graphene electrons are quantum. This approach is widely known and well-tested [6]. Note that the authors performed the complete classical solution of the problem, where all subsystems are considered classically. In the semi-classical approach, the derivation of the basic equation (and it coincides with the equation in the classical approach) is methodologically simpler.

In this paper, we study the features of three-dimensional extremely short pulse propagation in graphene taking into account an inhomogeneity. Here we mean the region of increased electron density. Such inhomogeneity can lead to the appearance of interesting and unexpected physical effects that are of practical importance. We noted earlier that effects with a completely different type of inhomogeneity were considered, namely, with varying electric field along the CNTs (carbon nanotubes) axis. In particular, the

work [7] is associated with two-dimensional modeling of the propagation of ultrashort electromagnetic pulses in an array of CNTs with a varying electric field along the axis. In addition, recently, the authors carried out a comprehensive study of the latter task in the 3D case, as a result of which the possibility of bipolar propagation of electromagnetic breathers through the array of CNTs was demonstrated, taking into account the varying electric field [8]. It was found that in this specific case, an electromagnetic pulse causes a significant redistribution of the electron density in the sample, both for 2D and 3D systems. In addition to the varying field leading to the redistribution of electrons, there are other natural inhomogeneities observed in experimental samples. Especially important problem occurs in the situation when inhomogeneities are caused by regions of increased concentration of conduction electrons due to the presence of impurities. In this regard, it seems appropriate to study the effect of electron concentration inhomogeneity on the propagation characteristics of extremely short electromagnetic pulses in graphene. The question of establishing the region of spatial inhomogeneity of carrier concentration in the form of an extremely short pulse is of most interest. The relevance of this issue is crucial for modern applications of optoelectronics. In this paper, we are interested only in the shape of the optical pulse and show that it changes. This can easily be measured using pre-existing autocorrelation techniques.

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2. STATEMENT OF THE PROBLEM AND BASIC EQUATIONS

Let's consider the propagation of extremely short electromagnetic pulses in graphene with impurities, with the electric field of the pulse directed along the x axis.

The electron spectrum of graphene obtained in the renormalization group approach is given according to [9] as:

$$\begin{aligned} \varepsilon(p_x, p_y) &= v(p_x, p_y) \sqrt{p_x^2 + p_y^2 + m^2} \\ v(p_x, p_y) &= \frac{\gamma_0}{\pi} \ln \left(\frac{\sqrt{p_x^2 + p_y^2 + m^2}}{\varepsilon_0} \right). \end{aligned} \quad (1)$$

Here, p_x, p_y are the electron's momentum components, m is the gap in the spectrum (0.1 eV) [9], γ_0 is the overlap integral (2.7 eV), ε_0 is the energy at which the velocity is measured (i.e., we use a system of units in which the Fermi velocity for electrons near the Fermi level is taken as unity). Here it is necessary to make the following comments. First, considered graphene has the gap in the energy spectrum, since the introduction of impurities, i.e. disturbances, leads to this effect. Second, the mode of scattering of graphene electrons is considered here according to [9] and in the approximations made in this work. The main difference from the previous considerations is the dependence of the Fermi velocity on the electron energy, to which the influence of impurities reduces. The fundamental point is the fact that the electromagnetic field is considered classically based on Maxwell's equations. This is due to the fact that the intensities of extremely short pulses are quite large (up to 10^7 V/cm) and, therefore, a pulse contains many photons, so that quantum effects associated with fluctuations in the number of photons can be neglected [10].

According to the quantum mechanics, in the presence of an external electric field E , which is directed along the x -axis and considered as $E = -\partial A/c\partial t$, we should change momentum on generalized momentum $\mathbf{p} \rightarrow \mathbf{p} - e\mathbf{A}/c$ (e is the electron charge).

Let's write the wave equation for 3D case in the cylindrical coordinate system:

$$\mathbf{A}_u = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \mathbf{A}}{\partial r} \right) + \frac{\partial^2 \mathbf{A}}{\partial z^2} + \frac{1}{r^2} \frac{\partial^2 \mathbf{A}}{\partial \varphi^2} + 4\pi \mathbf{j}(\mathbf{A}). \quad (2)$$

Further, we assume that $\partial/\partial\varphi \rightarrow 0$ due to the cylindrical symmetry.

Note also that the estimates made in [8] allow us to conclude that the effect of charge accumulation for femtosecond pulses can be neglected. This is confirmed by numerical experiments for the case of carbon nanotubes and a pulse of tens of femtoseconds in duration.

The standard expression for the current density can be written as:

$$\begin{aligned} \mathbf{j} &= e \sum_p v_y \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right) \langle \alpha_p^+ \alpha_p \rangle, \\ v_y(\mathbf{p}) &= \frac{\partial \varepsilon(\mathbf{p})}{p_y}, \end{aligned} \quad (3)$$

where parentheses mean averaging with a non-equilibrium density matrix. Operators a and a^+ relate only to the electronic subsystem, which does not contradict the presence of a sufficiently large number of photons in the pulse (there should really be about 50 in order for our approximation to work, and this will be linear, not a nonlinear mode like ours). In the expression for current density, we can use the number of particles that follows from the Fermi-Dirac distribution. Further, we will consider the case of low temperatures, when only a small region in the momentum space near the Fermi level contributes to the sum (integral). So, we write the formula (3) in the form:

$$\mathbf{j} = e \int_{z_B} dp_x dp_y v_y \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right) \quad (4)$$

The nonlinearity in equation (1) is a nonlinearity with saturation. In the case of taking into account the spatial inhomogeneity of the charge density, the equation for the propagation of an extremely short pulse can be written as:

$$\begin{aligned} \mathbf{A}_u &= \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \mathbf{A}}{\partial r} \right) + \frac{\partial^2 \mathbf{A}}{\partial z^2} + \frac{1}{r^2} \frac{\partial^2 \mathbf{A}}{\partial \varphi^2} + 4\pi \mathbf{j}(\mathbf{A}) \cdot f(z), \\ f(z) &= 1 - \alpha \cdot \exp \left(-\frac{(z - z^*)^2}{\delta} \right). \end{aligned} \quad (5)$$

Here, $f(z)$ is the function that determines the spatial inhomogeneity of the charge density, α and δ are the depth and width of the spatial inhomogeneity, respectively, z^* is the position of the displacement of the inhomogeneity. The term with the derivative with respect to the angle φ can be neglected in the future due to symmetry. Note that the reduced form of nonlinearity is characteristic of graphene. For a different kind of nonlinearity, there will be different results.

3. RESULTS OF NUMERICAL SIMULATION

The equation (5) is solved numerically [11]. The initial condition has the form:

$$\begin{aligned} \mathbf{A}(z, r, 0) &= Q \exp \left(-\frac{(z - z_0)^2}{\gamma_z^2} \right) \exp \left(-\frac{r^2}{\gamma_r^2} \right) \\ \frac{d\mathbf{A}(z, r, 0)}{dt} &= 2v_z Q \frac{z - z_0}{\gamma_z^2} \exp \left(-\frac{(z - z_0)^2}{\gamma_z^2} \right) \exp \left(-\frac{r^2}{\gamma_r^2} \right) \end{aligned} \quad (6)$$

where r is the radius, Q is the pulse amplitude ($2 \cdot 10^6$ V/m), γ_z, γ_r define the pulse width (400 nm, 450 nm), v_z is the initial pulse velocity in the z -direction (95 % from the light velocity), z_0 is the initial pulse center shift ($4 \cdot 10^3$ nm).

The pulse evolution is presented in Fig. 1.

This behavior of the pulse is associated with the type of nonlinearity in (5). There is a decrease in the amplitude of the pulse, as well as its spreading over time. That is, we can conclude about the instability of the pulses, which leads to a violation of their structure.

The dynamics of a 3D extremely short pulse with allowance for inhomogeneity is presented in Fig. 2.

As follows from Fig. 2, the introduction of spatial inhomogeneity of the charge density does not prevent the pulse from spreading along the transverse coordinate,

but counteracts a significant decrease in the amplitude of the pulse.

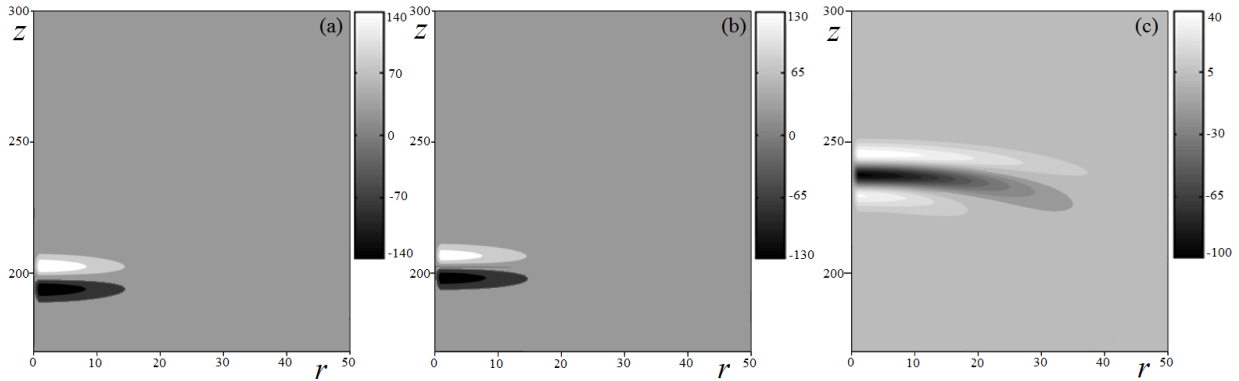


Fig. 1 – The electric field strength of 3D electromagnetic pulse (one unit corresponds to 10^6 V/m) at different time points: (a) the initial pulse; (b) $t = 0.5 \cdot 10^{-13}$ s; (c) $t = 5.0 \cdot 10^{-13}$ s. The unit along the r -axis corresponds to 30 nm, along the z -axis – 20 nm

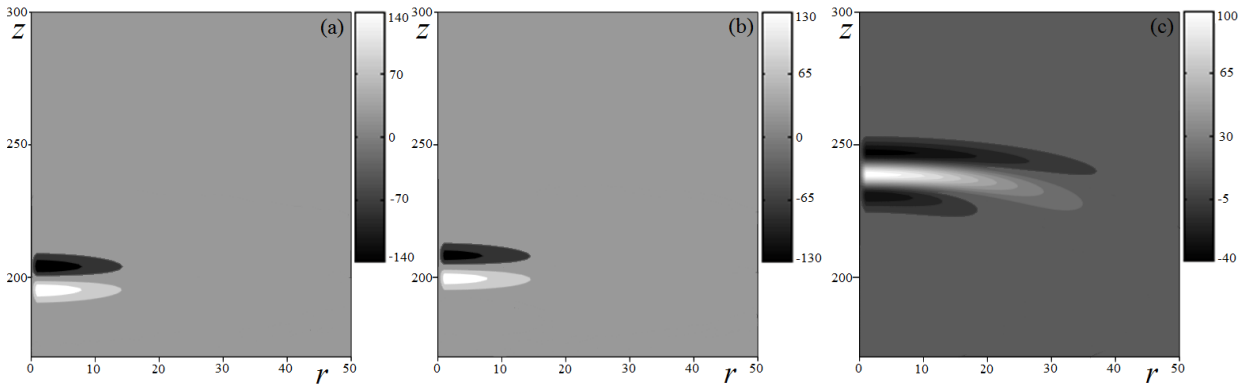


Fig. 2 – The electric field strength of 3D electromagnetic pulse (one unit corresponds to 10^6 V/m) at different time points, taking into account the heterogeneity ($\alpha = 0.8$ r.u., $\delta = 5$ r.u.): (a) the initial pulse; (b) $t = 0.5 \cdot 10^{-13}$ s; (c) $t = 5.0 \cdot 10^{-13}$ s. The unit along the r -axis corresponds to 30 nm, along the z -axis – 20 nm

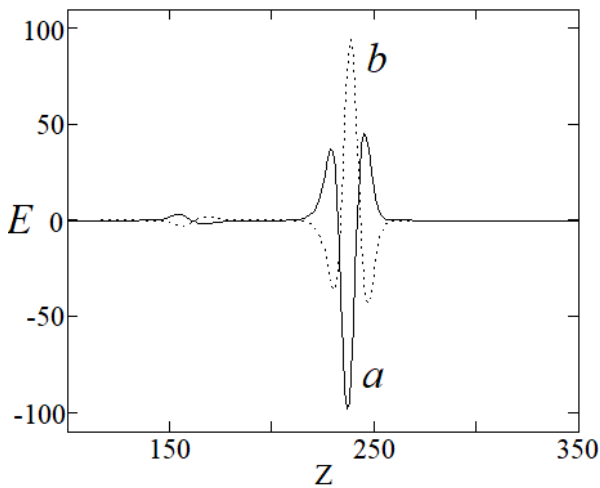


Fig. 3 – Comparison of the electric field strengths of a 3D electromagnetic pulse (one unit corresponds to 10^6 V/m) in the case of taking into account inhomogeneity (b) and without it (at $t = 5.0 \cdot 10^{-13}$ s): (a) without inhomogeneity; (b) $\delta = 5$ r.u. The unit along the r -axis corresponds to 30 nm, along the z -axis – 20 nm

Comparison of cases with and without spatial inhomogeneity is shown in Fig. 3.

According to the calculation results, approximately

the same spreading of the pulse occurs in the case of homogeneity and without it. However, in the case of introducing spatial inhomogeneity of the charge density into the medium, the loss of pulse in the amplitude is minimized compared with the case of a homogeneous medium. Note also that the width of the introduced inhomogeneity does not have a significant effect on the nature of the propagation of an extremely short pulse in graphene. Numerical calculations have shown that the depth of spatial inhomogeneity also has a weak effect on the pulse shape.

4. CONCLUSIONS

The main results of this work are the following:

1. 3D extremely short optical pulses propagate unstably with violation of the pulse shape.
2. The introduction of the spatial inhomogeneity of the charge density into the medium makes it possible to reduce the loss of the pulse amplitude.
3. The depth of the spatial inhomogeneity of the charge density does not have a noticeable effect on the pulse shape.
4. All the predictions made and the consequences arising from them (technical applications can be used in the control and management of the form of extremely short pulses) are based on a semi-classical approach.

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Тривимірні надзвичайно короткі оптичні імпульси в графені з неоднорідностями

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Розглядаються рівняння Максвелла для електромагнітного поля, що поширюється у домішковому графені з урахуванням просторової неоднорідності. Під гетерогенністю мається на увазі наявність області підвищеної електронної щільності. Особливо важливим випадком є неоднорідність, яка обумовлена ділянками підвищеної концентрації електронів провідності внаслідок наявності домішок. Згідно з цим фактом представляється доцільним дослідити вплив такої неоднорідності на поширення імпульсу в домішковому графені. Внаслідок різноманітності домішок і характеру їх взаємодії з підсистемою графена у таких задачах можливі різні підходи. Один із них полягає у розгляді розсіяння балістичних електронів у графені домішками. Домішки вважаються відповідальними за виникнення розупорядкування і слабкої локалізації. У цьому випадку вони виходять за межі самоузгодженого наближення Борна і застосовується підхід до перенормування. У даній роботі електронний спектр для підсистеми графена взято з підходу групи перенормування, широко використовуваного у квантовій теорії поля, коли перехід від ділянок з меншою енергією до ділянок з більшою енергією обумовлений зміною масштабу системи. Основна ідея полягає у тому, що швидкість Фермі перенормується і починає залежати від енергії електронів логарифмічно. У рамках напівкласичного підходу отримано ефективне рівняння для векторного потенціалу електромагнітного поля, яке розв'язане чисельно. Виявлено, що тривимірні надзвичайно короткі оптичні імпульси розповсюджуються із порушеною формою імпульсу. При цьому введення просторової неоднорідності щільності заряду у середовище дозволяє зменшити втрати імпульсу в амплітуді. Досліджено вплив просторових параметрів неоднорідності на картину розповсюдження надзвичайно короткого оптичного імпульсу. Показано, що глибина і ширина просторової неоднорідності щільності заряду не мають суттєвого впливу на форму імпульсу.

Ключові слова: Ультракоткий імпульс, Графен, Неоднорідність, Щільність заряду.