Amplification of a Few Cycle Optical Pulses in Graphene

Natalia Yanyushkina, Mikhail Belonenko, and Nikolay Lebedev

Abstract—This paper focuses on the propagation of a few cycle optical pulses in graphene in the case of electromagnetic field. Electrons in the quantum formalism were considered and a change of dispersion law with Coulomb repulsion was taken into account. The effective equation was numerically analyzed and an influence of Coulomb repulsion was found. The amplification of few cycle optical pulses in graphene with applying of electromagnetic field to our system was discovered. Results about the amplification of pulse in graphene have been achieved.

Index Terms—Colomb repulsion, few cycle optical pulses, Maxwell equations.

doi: 10.3969/j.issn.1674-862X.2010.01.010

1. Introduction

Great interests in the nonlinear phenomena have been recently stimulated to create the materials with nonlinear properties under easy available experimental conditions. One of such materials is a carbon nanotube—a structure which consists of one layer of carbon atoms, locates in the units of hexagonal lattice and is rolled into a cylindrical shape. Great attention is paid to a large electron mobility in the carbon nanotubes and to its unique property which is an alternative of silicic base in the up-to-date microelectronics[1]-[4].

As it is well known, electromagnetic waves in the carbon structures become strongly nonlinear even in the weak fields which give rise to spread possibility of solitary electromagnetic waves in the graphene and carbon nanotubes. These properties of carbon nanostructures are of theoretical interest and have been considered to apply in the nonlinear optics[5],[6].

The electron subsystem is often described with Boltzmann kinetic equation in approaching constant relaxation time but it requires microscopic explanation. An alternative way is electron dynamics described with a complex dispersion law in the microscopic approach which is based on Hamiltonian system only[7]. It is also effective for low temperatures. Nevertheless, we should note that it is not often attended to electronic properties, which can be shown in the optical spectrum. For example, Coulomb electron interaction can lead to a change of dispersion law and thereby to a change of optical response.

It is worth to note that the simplest way is to take Coulomb interaction into account in the Hubbard model[8],[9]. In this paper, we will consider the influence of electromagnetic field which can affect the pulses dynamics.

2. Basic Equations

Considering a spread of plane-polarized electromagnetic pulse in geometry when its wave-vector is perpendicular to graphene layers and the polarization vector is along \( x \) axis as shown in Fig. 1, the electronic states in consideration can be described by the Hubbard model[8],[9]:

\[
H = H_0 + H_{\text{int}}
\]

\[
H_0 = \sum_{j,\sigma} t_0 \hat{a}_j^{\dagger} \hat{a}_{j+\Delta} + c.c.
\]

\[
H_{\text{int}} = U \sum_j \hat{a}_j^{\dagger} \hat{a}_{j,\sigma} \hat{a}_{j,-\sigma}^{\dagger} \hat{a}_{j,-\sigma} + c.c.
\]

where \( \hat{a}_{j,\sigma}^{\dagger} \) and \( \hat{a}_{j,\sigma} \) are Fermi operators of creation and annihilation of electrons (\( j \) and \( \sigma \) are space and spin indexes respectively); \( t_0 \) is jumping integral (resonance integral); \( \Delta \) is vector which bonds adjacent lattice units; \( U \) is Coulomb’s repulsion of electrons in the same unit.

We can obtain the electron spectrum describing the properties of electron subsystem without Coulomb repulsion \( \Delta(p) \) using a Fourier transform:

![Fig. 1. Geometry of graphene layers and polarization vector.](image-url)
\[
a_{n,s}^{-} = \frac{1}{N^{1/2}} \sum_{j} a_{j,n,s} \exp(in) \\
a_{n,s}^{+} = \frac{1}{N^{1/2}} \sum_{j} a_{j,n,s} \exp(-in)
\]

where \(i\) is imaginary unit and \(n\) is index in momentum space.

The spectrum of elementary excitations can be used in the model changes if the term \(U\) is taken into account. Therefore, two originally degenerating zones are broken up into two non-degenerating zones with the following spectrum:

\[
\epsilon_{p}(p) = \epsilon(p)^{2}/2 + V_{p}(1 - V_{p}) + U_{g}^{2}/2
\]

where \(n_{0}\) is the concentration of the electrons in the thermal equilibrium in the graphene, \(p\) is momentum which is directed along the axis \(z\), and \(a(p)\) is defined by

\[
\epsilon(p) = \pm \sqrt{1 + 4 \cos(\epsilon_{p}) - 2 \epsilon_{p}(1 - V_{p}) + U_{g}^{2}/2}
\]

where \(\gamma \approx 2.7\) eV, \(a = 3h/2\) (\(h = 6.582 \times 10^{-16}\) eV \(\cdot s\) is the Planck’s constant), \(b = 0.142\) nm is the distance between adjacent carbon atoms in the graphene. Different signs are treated to conductance zone and valence zone. Equation (4) is the dispersion law describing graphene properties without Coulomb interaction of electrons in the one unit.

Furthermore, considering electric field spread in the directions orthogonal to the propagation axis \(z\), we can write a standard expression for the current density in an electromagnetic field of high-frequency field and substituting the averaging result into (6), we obtain

\[
\mathbf{J}_{0} = e \sum_{p,r} \left\{ p - \frac{e}{c} \mathbf{A}(t) - \frac{e E_{0}}{w_{0}} \cos \omega_{p} t \right\} \langle a_{p,r}^{+} a_{p,r} \rangle
\]

where \(\mathbf{J}_{0}\) is the density of current.

Now neglecting the diffraction blooming of the laser beam in the directions orthogonal to the propagation axis \(z\), we can write a standard expression for the current density in the form:

\[
\mathbf{J}_{0} = e \sum_{p,r} \mathbf{v}_{r} \left( p - \frac{e}{c} \mathbf{A}(t) - \frac{e E_{0}}{w_{0}} \cos \omega_{p} t \right) \langle a_{p,r}^{+} a_{p,r} \rangle
\]

\[
\mathbf{v}_{r} = \sum_{p} D_{r,s} \sin(r \mathbf{p})
\]

where \(D_{r,s}\) is coefficient of the Fourier transform and \(r\) is a number of Fourier harmonics, then

\[
\mathbf{v}_{r} \left( p - \frac{e}{c} \mathbf{A}(t) - \frac{e E_{0}}{w_{0}} \cos \omega_{p} t \right)
\]

Now considering the pulse time \(\tau_{\text{imp}}\):

\[
\frac{2 \pi}{w_{0}} \ll \tau_{\text{imp}} \ll \tau_{\text{rel}}
\]

where \(\tau_{\text{rel}}\) is the relaxation time of electromagnetic field in the carbon nanotubes system; \(\tau_{\text{rel}} \approx 10^{-12}\) s and (8) is carried out, if \(\tau_{\text{imp}}\) is about \(10^{-12}\) s to \(10^{-11}\) s; \(w_{0}\) is the rate of high-frequency field\(^{(11)}\), which is about \(2 \pi \cdot 10^{14}\) s\(^{-1}\) to \(2 \pi \cdot 10^{15}\) s\(^{-1}\), and averaging (7) at the vibration period of high-frequency field and substituting the averaging result into (6), we obtain
\[ j_0 = -en_0 \sum B_s \sin \left( \frac{rc}{c} A(t) \right) \]  \hspace{1cm} (9a)\\
\[ B_r = C_r(\mathbf{E}_0) \sum_{s=1}^{\infty} \int_{-\varepsilon}^{\varepsilon/a} D_{rs} \cos(rp) \frac{\exp(-\beta c_r(p))}{1+\exp(-\beta c_r(p))} dp \]  \hspace{1cm} (9b)\\
\[ C_r(\mathbf{E}_0) = \frac{w_0}{2\pi} \int_{-\infty}^{+\infty} \cos \left( \frac{reE_0 \cos \omega t}{w_0} \right) dt \]  \hspace{1cm} (9c)

where \( B_r \) and \( C_r \) are expansion coefficients for current density \( j_0 \), and \( \beta = 1/(kT) \). After non-dimensionalizing of (5), we can get

\[ \frac{\partial^2 B}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 B}{\partial t^2} + \text{sgn}(B) \sin(B) \sum_{r=2}^{\infty} B_r \sin(rB) \|B_r\| = 0 \]  \hspace{1cm} (10)

where \( B \) is an amplitude of vector \( B \), \( B_r \) the expansion coefficient for current density \( j_0 \) when \( r=1 \) from (9a), and

\[ B = \frac{ea}{c}, x' = \frac{ea}{c} \sqrt{8\pi}, t' = \frac{ea}{c} \sqrt{8\pi n_0} \|B_r\|. \]

Note that (10) is just a generalization of the well-known Sine-Gordon equation in the case where the linear potential could be explained into the Fourier series. We reach the calculation that the dependence of this potential on the temperature, which determines the properties of the nonlinear solutions, is weak.

In the sum of (10) one can keep only several nonzero summands, since the coefficients \( b_r \) decrease with the increase of \( k \). In this way, one can obtain an analog of the double Sine-Gordon equation\(^{[12]} \), which is widely used. This equation cannot be solved in view of the method of the inverse scattering problem. The important consequence of this equation can be formulated as the theorem of “areas”.

The theorem says that only such pulses are stable with respect to a change of their form, when they have a certain “area” (“area” of the pulse \( \psi(t) \) is determined as

\[ \int_{-\infty}^{\infty} \psi(t)dt \].

The pulses of large “areas” tend to decrease it to reach the fixed value and those of a smaller “area” tend to increase it.

Another consequence of the double Sine-Gordon equation\(^{[12]} \) is that for fast decreasing boundary conditions, the properties of the interaction of the pulses and, what is more important, the decay characteristics of the solitary pulse strongly depend on its velocity. For increasing in the velocity, the pulses interact with a large elasticity and a smaller portion of their energy is transferred to the vibration modes.

All mentioned above stimulate the further numerical investigation of (10).

### 3. Results of Numerical Calculations

The equations were solved numerically by using a direct difference scheme of the cross type\(^{[13]} \). Steps of time and coordinate were determined, in view of the standard stability conditions. The difference scheme steps were halved sequentially, as long as the solution was not changed in the 8th significant digit. The initial condition was selected in the form of a well-known kink-solution of the sine-Gordon equation:

\[ B(x,t) = Q \cdot \text{arcctg} \left\{ \exp \left[ (x-vt)/\gamma \right] \right\} \]

\[ \gamma = (1-v^2)^{-1/2} \]

where \( Q \) was pulse amplitude. This initial condition corresponds to the case where an extremely short pulse was applied to the sample (The duration of pulse is a half of the electric-field oscillation period). In our calculations the following parameters, such as \( \gamma, b \), were chosen and estimated by quantum-chemical method modified neglecting of differential overlap method (MNDO)\(^{[14]} \).

The pulses evolution of electromagnetic field is defined by a sign of

\[ C_1(\mathbf{E}_0) = \frac{w_0}{2\pi} \int_{-\infty}^{+\infty} \cos \left( \frac{eE_0 \cos \omega t}{w_0} \right) dt \]

and for the case \( C_1(\mathbf{E}_0)<0 \) (inverted surroundings), it is given in Fig. 2.

It is observed that ultra cycle pulse is divided into a few pulses with different amplitude. Note such behavior was observed in the research of the analog of the Sine-Gordon equation in another nonlinear systems\(^{[9]} \) and it corresponds to carbon nanotubes systems\(^{[15]} \).[16]

The few cycle pulse is amplified and it gets a failing area. This fact is associated with our system that can be described in the frames of the double Sine-Gordon equation for which it is analog of the theorem of “areas”\(^{[15]} \).

![Fig. 2. Dependence of the electric field determined by (10) on the distance (from the initial point, where the pulse begins to propagate, to the given point): (a) at the time \( t=1 \), (b) at the \( t=2 \), and (c) at the \( t=3 \) (Time is in dimensionless units). The ratio \( v/c=0.95 \).](image)
Dependence of the amplified pulse form on the initial amplitude $Q$ is presented in Fig. 3. This dependence is accorded with the theorem of “areas” for Sine-Gordon equation, and a weak influence of initial amplitude on the exit amplitude is associated with nonintegrable summands in (10). Dependence of the amplified pulse form on the $E_0$ is given in Fig. 4. Note that a weak difference of results for the electromagnetic pulse amplitude is associated with non-dimensionalizing of equation system. The comparison results of two cases with amplification and without amplification are presented in Fig. 5.

The results of numerical calculations show that potential $U$ and the concentration of equilibrium electrons in the graphene $n_0$ have a weak influence on the form of the amplified pulse.

Note that considerable effect can have important practical applications. So, duration of the amplified few cycle pulse corresponds to terahertz frequencies and therefore we can obtain pulse amplification by illuminating from the beneath of graphene with laser emission.

4. Conclusions

In this paper, the following main results are achieved:

1) The effective equation for the dynamics of the electromagnetic field in the graphene with Coulomb interaction of the electrons in the low temperature case was obtained.

2) The possibility of the few cycle pulses amplification due to interaction with high-frequency field was shown.

3) Initial perturbation is divided on a few pulses. Part of them move in the opposite direction to the direction of the pulse with maximum amplitude.

4) Magnitudes of $U$ and $n_0$ have a weak influence on the form of the amplified pulse in the graphene.

5) It was shown by the numerical model that the few cycle pulses can stably spread in the graphene, so it is possible to use the graphene in the facilities for the few cycle pulses amplifications.

References


Natalia Yanyushkina was born in Volgograd, Russia, in 1986. She received the specialist degree from the Volgograd State University in Russia (VolSU), Volgograd, in 2008. She is currently pursuing the Ph.D. degree with the Department of Theoretical Physics and Wave Processes, Russia. Her research interests include few cycle optical pulses, Anderson model and Green’s technique.

Mikhail Belonenko was born in Volgograd, Russia, in 1966. He received the specialist degree from the Kazan State University in Russia (KSU), Kazan, in 1987. He received the Ph.D. degree from the KSU, Russia, in 1999 and professor from the Saratov State University (SSU), Russia, in 1998, both in physics. He is a professor with the Nanotechnology Laboratory in Volgograd Institute of Business, Volgograd, Russia. His research interests include few cycle optical pulses, CNTs, graphene, and ferroelectrics.

Nikolay Lebedev was born in Volgograd, Russia, in 1964. He received the specialist degree from VolSU, Volgograd, in 1985. He received the Ph.D. degree from the VolSU, Russia, in 1995 and professor from the Institute of Biochemistry Physics Russian Academy of Science (IPCP RAS), Russia, in 2006, both in chemical physics. He is a professor with the Department of Theoretical Physics and Wave Processes, Russia. His research interests include physical properties of carbon nanotubes and graphene, adsorption, Hubbard and Anderson models, and nonlinear effects.