In the manuscript

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LIGHT BULLETS IN THE BRAGG ENVIRONMENT WITH A CARBON NANOTUBES

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ABSTRACT
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Doctor of Physical and Mathematical Sciences

GENERAL DESCRIPTION OF WORK

The urgency of the problem. The main direction of development of physics in the XXI century, a physics of low-dimensional semiconductor, including nano-sized structures. In such structures, the elementary particle movement is restricted in two dimensions or less, so the size quantization occurs, in consequence of that, there are a number of unique physical and chemical phenomena. Thus the development of the physics of nanostructures is the next logical step in the development of high-tech production.

A special place in these studies took nanostructures based on carbon. One of the main advantages of carbon nanostructures is that changing the size and geometry of objects it is possible to control the conductive properties of the system [1, 2], as well as its optical properties, which is extremely important for the development of advanced optical applications.

In recent years, more and more scientific research group draws different durations of pulse propagation in an artificially simulated environments, such as photonic crystals, Bragg gratings [3], the left optical media, etc.

Carbon-based nanostructures, including carbon nanotubes, graphite, etc., are suitable environment for propagation of extremely short optical pulses [4-8]. This was considered the spread of extremely short pulses in the nanotube system in the presence of an external magnetic field and pulses encounter an array of semiconducting nanotubes. Also of interest is the proliferation of discrete solitons in waveguide structures based on pure and doped graphene and carbon nanotubes.

In this paper we consider the so-called Bragg (slotted) solitons [9-11]. Because the medium has a periodically alternating refractive index of the light pulse is distributed therein more slowly than in any fixed medium refractive index. This makes it possible to build on the basis of such media optical delay line, which find important applications, for example in the femtosecond spectroscopy.

The aim is to study the possibility of the existence and characteristics of the dynamics of light bullets in Bragg environment from carbon nanotubes. Achieving this goal involves the following tasks:

1. Modelling carbon structures for the study of propagation of extremely short optical pulse in a Bragg environment with carbon nanotubes.
2. The study of propagation of extremely short optical pulse in the external magnetic and electric field in a Bragg environment with carbon nanotubes.
3. Investigation of the effect of the Bragg grating on the interaction of two extremely

short optical pulses in a collision.

4. The study of two-dimensional propagation of extremely short pulses (light bullets) in Bragg environment with carbon nanotubes.

Scientific novelty. In this thesis the following results were obtained for the first time:

1. The effective dynamics equation for extremely short optical pulses, in case of the spatially modulated refractive index of the medium in which carbon nanotubes are placed.
2. Demonstrate the effect of the recovery waveform in an external electric field and its distortion in a magnetic field.
3. The possibility of the spread of discrete solitons in Bragg environment and control the shape of an extremely short pulse.
4. It has been found stable two-dimensional propagation of ultrashort pulses in a Bragg environment and confirmed that they carry information about the environment.

Research methods and the accuracy of the results. The reliability of the main provisions and conclusions of the thesis is provided by using a rigorous mathematical apparatus of theoretical physics, a thorough analysis of the physical principles and modeling, testing general algorithms based on the results obtained for particular cases, the coincidence of the results obtained by different methods, both qualitative and quantitative comparison with the existing experimental data, comparing already analyzed and substantiated findings and conclusions.

The scientific and practical value of the work. The thesis studied the processes of propagation of extremely short optical pulses in a medium with a spatially modulated refractive index based on carbon nanotubes, which are interesting not only from a fundamental point of view but also in terms of possible applications. The possibility of the spread Bragg (slot) solitons, discrete solitons, as well as two-dimensional light bullets in the Bragg grating with carbon nanotubes. These results open the possibility of creating new promising optical media, with which you can handle and manipulate optical signals, optical delay lines, which find important applications in microscopy and femtosecond etc., the results obtained can be used for modeling waveguides based on carbon nanotubes .

On defense are made the following provisions:

1. Distribution of extremely short optical pulse in a Bragg stable environment with carbon nanotubes. Extremely short optical pulses collide elastically at speeds close to the speed of light in the medium.

2. Under the influence of a constant electric field pulse narrowing slightly depending on the type of carbon nanotube and is determined by the external constant electric field.
3. Two-dimensional extremely short optical pulses (light bullets) spread steadily in Bragg environment and carry information about it.

Testing results. The results obtained in the thesis, presented at various conferences and seminars such as: the 14th All-Russian school seminar "Wave phenomena in heterogeneous environments," the memory of Professor AP Sukhorukov (Moscow region, village Krasnovidovo, 26-31 May 2014..); international Conference Imaginenano: Bringing together Nanoscience&Nanotechnology (Bilbao, Spain, 10-13 March 2015), XXVII Symposium "Modern chemical physics" (Tuapse, boarding house "Lighthouse", 20 September - 1 October 2015); XII International Workshop on Quantum Optics (IWQO-2015) (Moscow, Troitsk, Russia, 11-16 August 2015); and conferences and scientific seminars in the "Volgograd State University."

Personal contribution of the author. Thesis content reflects the author's personal contribution to the published work. Statement of the problem, the choice of directions and methods of research conducted by the author together with the supervisor. The bulk of the theoretical calculations carried out directly by the author, and the analysis and interpretation of the results of calculations carried out in collaboration with the supervisor Prof. MB Belonenko.

The structure and scope of the thesis. The thesis consists of an introduction, five chapters, conclusion and bibliography of 138 titles, containing 111 pages of text, 40 pictures.

Papers. According to the results of the research published 6 works, including 4 articles in journals from the list of RF HAC.

HIGHLIGHTS OF WORK

In the introduction the urgency of the work, formulated the goal, objectives of the study and the provisions for the defense.

The first chapter of "literature review" provides an overview of scientific publications devoted to the study of the structure and properties of carbon nanotubes. Attention is paid to the review of studies of spatial-temporal solitons, or the so-called light bullets. In the final part of the chapter deals with the history of development of spatial lattices with variable refractive index, such as Bragg gratings.

The second chapter "of extremely short optical pulses in Bragg

environment with carbon nanotubes" is devoted to the study of propagation of extremely short optical pulse in a Bragg environment with carbon nanotubes. The results of calculations of various collisions of extremely short pulses at various parameters Bragg environment, as well as in the presence of external electric and magnetic fields.

Research of electronic structure of CNT, held in the strong-coupling approximation in the analysis of the dynamics of π-electrons. The dispersion relation for zigzag CNT (m, 0) has the form [12]:

$$E(\mathbf{p}) = \pm\gamma\sqrt{1+4\cos(ap_z)\cos(\pi s/m)+4\cos^2(\pi s/m)}\ , \qquad (1)$$

где $\gamma = 2.7$ eV, $a = 3b/2\hbar$, $b = 0.152$ nm – the distance between adjacent carbon atoms, and ***p*** is defined as quasi-momentum (p_z, s), $s = 1, 2 \ldots m$.

In constructing the model, we will describe the electromagnetic pulse field on the basis of Maxwell's equations in the Coulomb gauge. The vector potential is of the form: $\mathbf{A} = (0,0,A_z(x,t))$

$$\frac{\partial^2\mathbf{A}}{\partial x^2} - \frac{n^2(x)}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} + \frac{4\pi}{c}\mathbf{j} = 0\ , \qquad (2)$$

where $n(x)$ defines the spatial variation of the refractive index, *j* - current, owes its appearance to an electric field pulse to the electrons in the conduction band of the nanotube. Here we ignore the diffraction spreading of the laser beam in the direction perpendicular to the axis of propagation, the electric field of the substrate, interband transitions. Since the typical size of the CNT and the distance between them is much smaller than the size of the spatial region in which localized extremely short pulse, you can use the approximation of a continuous medium and count the current distributed by volume.

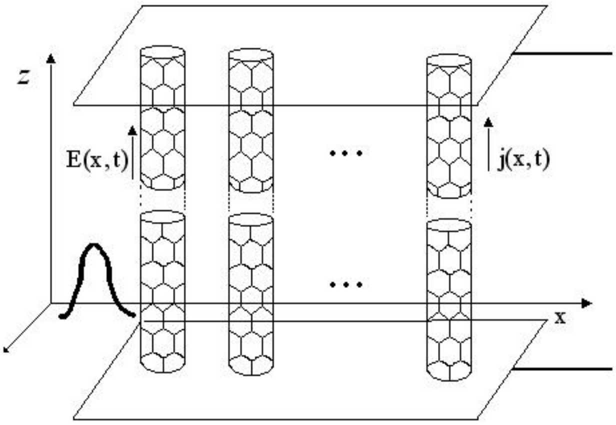

Fig. 1. The geometry of the problem, where *j(x t)* - current, along the nanotube axis, *E(x,t)* - the electric field pulse.

Since the typical relaxation time for electrons in the nanotube 10^{-13} s, the electron ensemble at times the typical problems of the dynamics of extremely short pulses (of the order 10^{-14} s) can be described with the help of the collisionless Boltzmann equation.

Finally, the effective equation can be written as:

$$\frac{\partial^2 A_z}{\partial x^2} - \frac{n^2(x)}{c^2}\frac{\partial^2 A_z}{\partial t^2} + \frac{q}{\pi\hbar}\sum_m c_m \sin\left(\frac{maq}{c}A_z(t)\right) = 0,$$

$$c_m = \sum_m a_{ms} b_{ms}, \quad b_{ms} = \int_{-q_0}^{q_0} dp_z \cos(map_z) F_0(\mathbf{p}), \qquad (3)$$

где $F_0(\mathbf{p})$ – equilibrium Fermi distribution function. As with increasing m coefficients c_m decrease, in the amount of (3), for evaluations may be only the first two terms and get double the equation sin-Gordon, from which it follows that the character of a single pulse of decay strongly depends on its velocity. With increasing speed pulses interact more elastic and less of their energy goes into the vibrational modes.

Equations (3) were solved numerically using the direct finite difference schemes such as the cross. The initial conditions on the vector potential:

$$A_{t=0} = A_0 \exp\left\{-\frac{x^2}{\gamma^2}\right\}, \quad \left.\frac{dA}{dt}\right|_{t=0} = \frac{2vx}{\gamma^2} A_0 \exp\left\{-\frac{(x-vt)^2}{\gamma^2}\right\} \qquad (4)$$

The refractive index of the medium: $n(x) = n_0(1 + \alpha\cos(2\pi x/\chi))$.

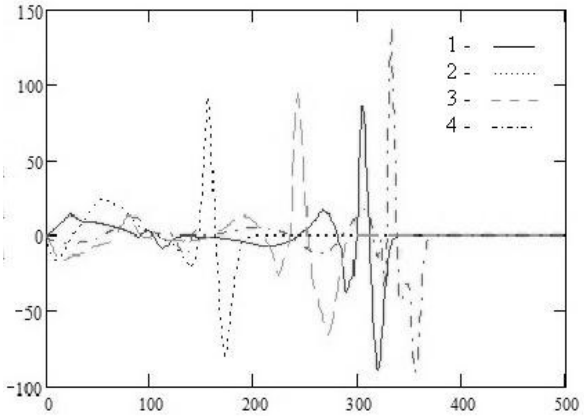

Fig. 2. Evolution of extremely short optical pulses at a fixed time T = 2,5 ps no Bragg grating (3); it (2); and at time points 2T (1) and 3T (4), if the lattice. The x-axis represents time in r.r., along the vertical axis in relative amplitude r.r.

Note that the lattice, as you might expect, leads to a distortion of the pulse shape due to the interference of the waves, experiencing partial "reflection." With the same due to interference and slower traveling pulse.

Chapter 3 "of extremely short optical pulses in Bragg environment with carbon nanotubes in external electric and magnetic fields" devoted to the study of propagation of extremely short pulses in Bragg environment with carbon nanotubes in the presence of external electric and magnetic fields.

For carbon nanotubes zig-zag type dispersion law of electrons in a magnetic field parallel to the nanotube axis is:

$$\varepsilon_s(k_x, k_y, H) = \pm\gamma\sqrt{1 + 4\cos\left(ap_z\frac{3ak_z}{2}\right)\cos\left(\frac{\sqrt{3}ak_x}{2}\right) + 4\cos^2\left(\frac{\sqrt{3}ak_x}{2}\right)}, \quad (5)$$

where a=1.4 Å, k_z– the wave vector along the axis of the tube, $k_x = \frac{2\pi}{\sqrt{3}aM_0}\left(s + \frac{\Phi}{\Phi_0}\right)$, Φ – the magnetic flux through the cross section of the nanotube, $\Phi_0 = \hbar c/e$, $s = 1, 2, \ldots, 2M_0$, M_0 – the number of hexagons on the nanotube perimeter.

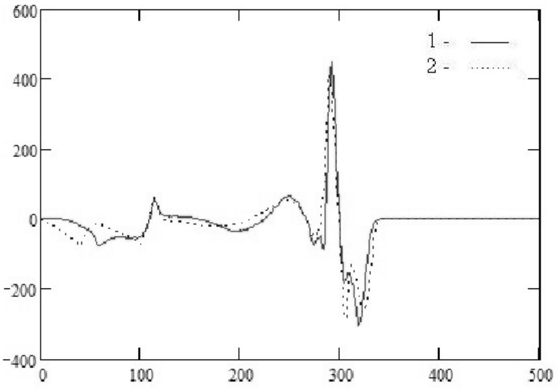

Fig. 3. Evolution of extremely short optical pulses at a fixed time t = 2.5 ps, in the presence of a Bragg grating in an external magnetic field (2) and without it (1). The x-axis represents time in rel. u, along the vertical axis in relative amplitude. u

Influence of the magnetic field is reduced to changing the shape of extremely short optical pulse due to changes in the dispersion relation, described by equation (5). The magnetic field applied parallel to the axis of the carbon nanotube, the dispersion law changes, which consequently affects the character of the "collapse" extremely short pulse and accordingly changes its shape (Fig. 3).

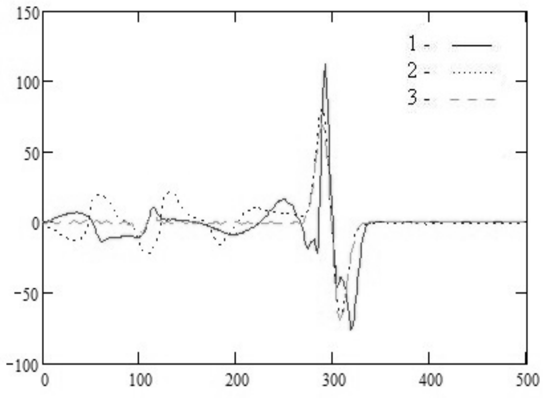

Fig. 4. The evolution of extremely short optical pulses at a fixed time T = 02.05 ps, in the absence of an external electric field (1) under the influence of the field (2) and a large field of 10 times (3). The x-axis represents time in rel. u, along the vertical axis in relative amplitude. u

The constant external electric field has a stabilizing effect and reduces the impulse of alternating electromagnetic field, compared with the case of absence of the constant field. This can be attributed to the fact that in the presence of a constant field in the electron spectrum a so-called "Stark ladder" and electrons can change its energy only by an amount proportional to the difference between the energy levels of the adjacent steps. This leads to a decrease in the effective dispersion of electrons, and thus, in turn, to reduce the dispersion spreading of the pulse of the alternating electric field. Starting with a certain value of the constant field pulse of alternating electric field ceases to be narrowed and is beginning to spread in the stationary mode. Qualitatively, this behavior can be explained by the competition between the processes of dispersion "collapse" of the pulse in the absence of the constant field and the movement of electrons on the "Stark ladder."

In the fourth chapter, "The proliferation of discrete solitons and two-dimensional light bullets in Bragg environment with carbon nanotubes" contains the results of calculations of evolution dikretnyh solitons, as well as distribution of two-dimensional light bullets in Bragg environments.

Maxwell's equation with the dielectric and magnetic properties of the system, taking into account calibration and can be written as:

$$\frac{\partial^2 \vec{A}_k}{\partial x^2} - \frac{n^2(x)}{c^2}\frac{\partial^2 \vec{A}_k}{\partial t^2} + \frac{4\pi}{c}\vec{j}_k - \frac{4\pi}{c}\frac{\partial \vec{P}_k}{\partial t} = 0 \qquad (6)$$

Here, the vector - potential $\vec{A}_k = (0,0,A_k(x,t))$ that corresponds to the electromagnetic field in the k-th layer consisting of CNTs, $\vec{j}_k$-current current in the k-th layer. $n(x)$ defines the spatial variation of the refractive index, i.e. Bragg grating, and $\vec{P}_k = \alpha(\vec{E}_{k-1} + \vec{E}_{k+1})$ - polarization induced in k-th layer and the electromagnetic field currents adjacent nanotubes. Note that below we assume the simplest model in which, where - coupling coefficient, and $\vec{E}_{k\pm1}$ - the value of the electric field.

We write the expression for the current density:

$$j_k = -en_0 \sum_l D_l \sin(\frac{le}{c} A_k(t))$$

$$D_l = \sum_{s=1}^{m} \int_{-\pi/a}^{\pi/a} dp_z B_{ls} \cos(lp_z) \frac{\exp(-\varepsilon_s(p_z)/k_B T)}{1 + \exp(-\varepsilon_s(p_z)/k_B T)}$$

(7)

where kB¬- Boltzmann's constant, T - temperature B_{ls} - coefficients of the expansion velocity of the charge carriers in a Fourier series:

$$v_s(p) = \sum_l B_{ls} \sin(lp_z)$$

$$B_{ls} = \frac{1}{2\pi} \sum_p v_s(p) \sin(lp)$$

Considering all of the above equation (6) after the dimensionless it can be represented as:

$$\frac{\partial^2 R_k}{\partial x'^2} - \frac{n^2(x)}{c^2} \frac{\partial^2 R_k}{\partial t'^2} - \mathrm{sgn}(D_1)\sin(R_k) - \sum_{l=2}^{\infty} (\frac{D_l}{|D_1|} \sin(lR_k)) + \frac{4\pi\alpha}{c} \frac{\partial^2 (R_{k-1} + R_{k+1})}{\partial t'^2} = 0$$

$$R_k = \frac{eA_k}{c}; x' = x\frac{2e}{c}\sqrt{\pi n_0 |D_1|}; t' = t\frac{2e}{c}\sqrt{\pi n_0 |D_1|};$$

(8)

The initial conditions on the vector potential wondered how:

$$A_{t=0} = A_0 \exp\left\{-\frac{x^2}{\gamma^2}\right\} \exp\left\{-\beta(N - N_c)^2\right\},$$

$$\left.\frac{dA}{dt}\right|_{t=0} = \frac{2vx}{\gamma^2} A_0 \exp\left\{-\frac{(x - vt)^2}{\gamma^2}\right\} \exp\left\{-\beta(N - N_c)^2\right\}$$

(9)

where *Nc*- central waveguide number (*Nc* = 6), *β* - parameter that determines the pulse width, *N* - number of the waveguide, t_0 - the start time.

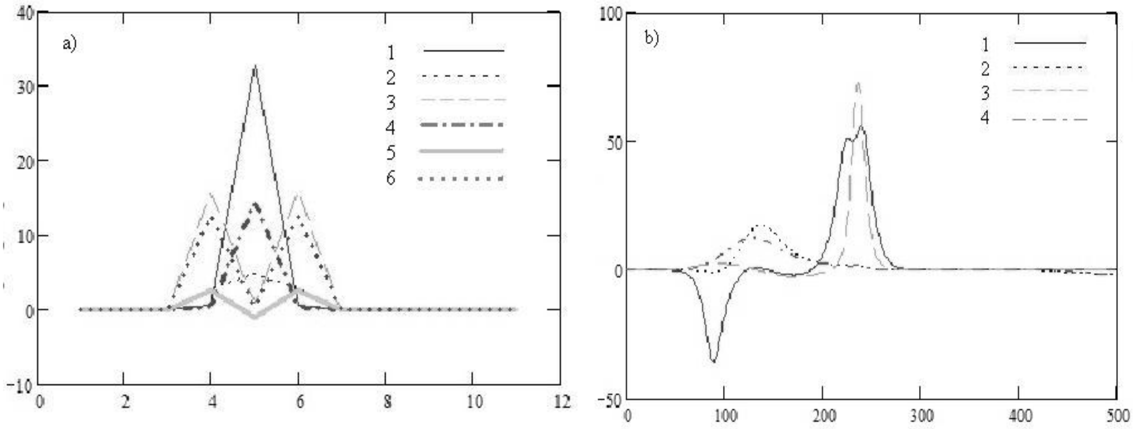

Fig. 5. The dependence of the electric field, the potential of the waveguide is determined number (Fig. A). The x-axis of the waveguide number N, the ordinate value of the dimensionless electric field. In the presence of the Bragg grating at times t = 2.5 ps (1a), t = 2 pixels (2a), t = 1.3 ps (3a); and without grating at times t = 2.5 ps (4a), t = 2 pixels (5a), t = 1.3 ps (6a). The dependence of the electric field changes over time (Fig. B). The x-axis of the dimensionless time, the ordinate value of the dimensionless electric field. In the presence of waveguides with Bragg gratings numbers N = 5 (1b), N = 6 (2b); and without grating waveguides numbers N = 5 (3b), N = 6 (4b).

From the Figure 5 shows that the pulses in a system with periodically varying refractive index slowed down, as required by the theory, and at the same time there is an exchange of energy between the different layers of the nanotube. Note that the energy (proportional to the square of the amplitude of the electric field is represented in the figure) partially "pumped" from the central layer of the nanotube to the neighboring and back. This energy exchange is typical for discrete solitons.

A pulse on the central waveguide hardly changes its shape depending on the initial pulse width unlike a pulse neighboring waveguides. On the side waveguides pulse has a tighter shape as the central, only a reduced amplitude. Changing the initial width of the main pulse, we can control the amplitude of the electromagnetic field on the adjacent waveguides. Moreover, the wider the system applied to the CNT pulse, the greater the amplitude of the neighboring central pulse. This in turn makes it possible to control the shape extremely short pulse by changing the number of layers and the CNT layer spacing that determines the coupling coefficient.

Basic equations and their solutions, describe the two-dimensional distribution of extremely short optical pulses (light bullets) in a medium with variable refractive index with carbon nanotubes shown in Chapter 2.

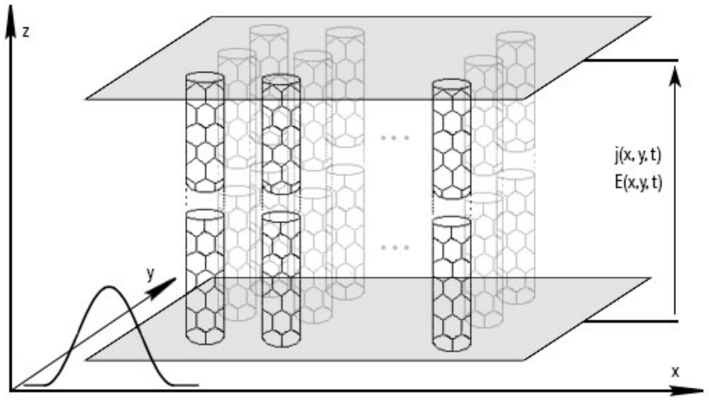

Fig. 6. The geometry of the problem, where f (x, y, t) - current, along the nanotube axis, E (x, y, t) - the electric field pulse**.**

The initial conditions on the vector potential were set as:

$$A(x,y,t=0)=A_0\exp\left\{-\frac{x^2}{\gamma^2}\right\}\exp\left\{-\beta(y-y_0)^2\right\},$$

$$\left.\frac{dA_z}{dt}\right|_{t=0}=\frac{2vx}{\gamma^2}A_0\exp\left\{-\frac{x^2}{\gamma^2}\right\}\exp\left\{-\beta(y-y_0)^2\right\} \tag{10}$$

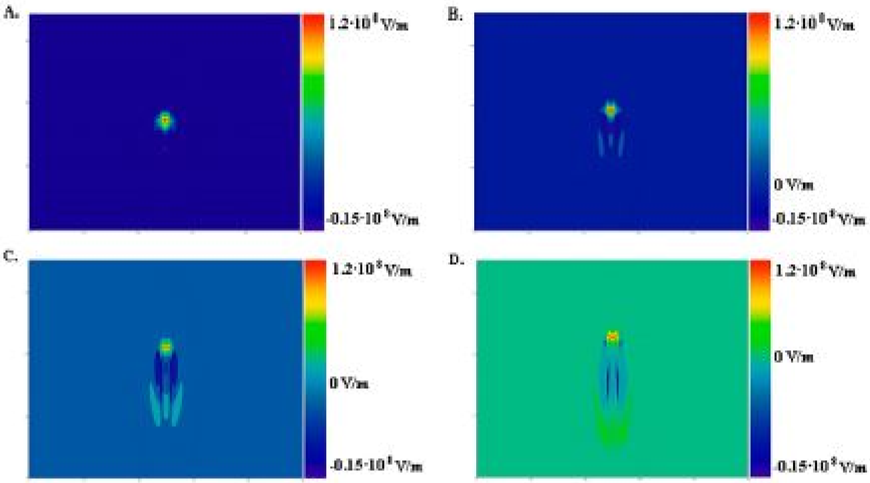

Fig. 7. Distribution of light bullets in Bragg environment with carbon nanotubes at a fixed time and) $t = T_0$, b) $t = 2\ T_0$ in) $t = 3\ T_0$, r) $t = 4\ T_0$, where $T_0 = 2.5 * 10^{-12}$ c - initial period light bullets. The values of the field strength are shown on a color scale, the maximum values correspond to the red area, and the minimum - purple.

As can be seen from the evolution of the two-dimensional propagation of extremely short optical pulses (Fig. 7), it changes its configuration a few, there is an effect of spreading shape over time due to dispersion effects.

The solution for the two-dimensional light bullets in Bragg environment remains localized, but changes due to lateral dispersion, its spatial structure. The combined effect of the spreading effects of momentum due to the dispersion and nonlinearity leads to the formation of multi-peak transverse structure, which nevertheless remains localized in a bounded spatial domain.

In the fifth chapter, "Two-dimensional light bullets in an environment with cross-modulated refractive index" contained the results of studies of propagation of light bullets in Bragg systems with different spatially modulated refractive indices.

The refractive index of the medium was modeled as:

$n(x) = n_0(1+\alpha\cos(2\pi x/\chi))(1+\Delta^2(y-y_0)^2)$, where α - the modulation depth of the Bragg grating, χ, Δ - lattice periods in the respective direction.

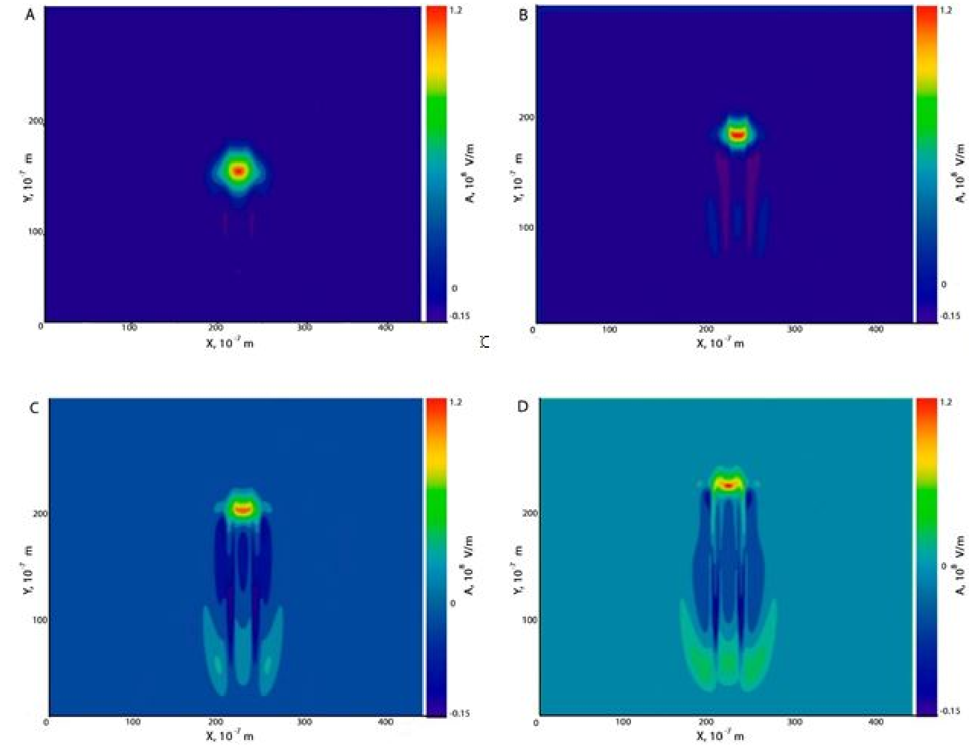

Fig. 8. Distribution of light bullets in Bragg environment with cross modulation (grating period χ = 2.5 microns) with carbon nanotubes at a fixed time a) T = 2.5 ps, b) 2T c) 3T, d) 4T. The axes are the relative coordinates and the electric field unit.

The refractive index of the medium at a harmonic modulation:

$$n(x) = n_0\left(1+\alpha\cos(2\pi x/\chi)\sin((y-y_0)^2\Delta^2)\right).$$

As can be seen from the obtained dependency (Fig. 9) in a light bullet Bragg cross modulation medium with a refractive index not experience broadening, but there are electric oscillations in the medium after its passage. We attribute this to the lack of balance between the environmental dispersion and nonlinearity of the medium (in contrast to the case of solitons) thereby form a light bullet changes. We also note that, despite the change in the form of light energy of the bullet is still concentrated in a limited area. Due to the modulation of the refractive index in the transverse direction to the axis of propagation has reduced feathering in this direction, due to the dispersion. The combined effect of the spreading effects of momentum due to the dispersion and nonlinearity leads to the formation of multi-peak transverse structure, which nevertheless remains localized in a bounded spatial domain.

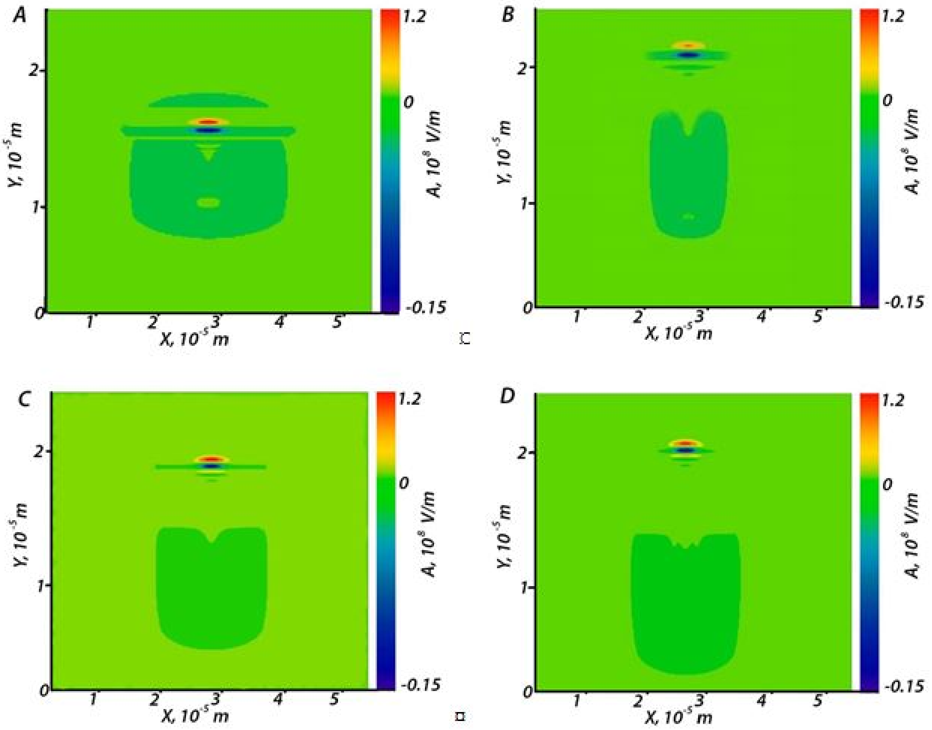

Fig. 9. Distribution of light bullets in Bragg environment harmonic modulation (grating period x = 2.5 mm) with carbon nanotubes at a fixed time a) T = 2.5 ps, b) 2T in) 3T, g) 4T. The axes are the relative coordinates of the unit and the electric field.

Finally, it is the most important results and conclusions of the thesis.

KEY FINDINGS AND RESULTS

1. Distribution of extremely short optical pulse in a Bragg stable environment with carbon nanotubes, with the distortion of its shape. It was found that the lattice constant and the refractive index modulation depth affects the speed of propagation of extremely short pulses and its shape.

2. When increasing the pulse rate value decreases their spatial localization, and the collision time, this leads to the fact that the elastic facing pulses, although with a significant change in shape due to the interaction with the Bragg grating.

3. Propagation of the short optical pulse is stable in medium in the presence of Bragg external magnetic and electric fields. The presence of the electric field has a stabilizing effect and reduces the impulse of alternating electromagnetic field, compared with the case of absence of the constant field.

4. It was found that the distribution of discrete solitons and two-dimensional light bullets steadily in Bragg environment with carbon nanotubes. The existence of the possibility to control the speed of propagation of light bullets, changing the parameters of the Bragg grating.

5. Dynamics of light bullets in an environment with an additional transverse and harmonic modulation of the refractive index is similar to Bragg, but there are power fluctuations in the environment after its passage through the lattice.

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