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# MODELING OF TWO-DIMENSIONAL LIGHT BULLETS PROPAGATION IN AN ARRAY OF CARBON NANOTUBES TAKING INTO ACCOUNT THE MECHANICAL TENSION AND MAGNETIC FIELD [1]

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**Abstract.** In this paper, we study the influence of acoustic and magnetic fields on the propagation of the two-dimensional light bullet in an array of carbon nanotubes. The acoustic field is taken into account in the framework of the gauge theory. A magnetic field is applied along the nanotube axis and leads to a change in the electronic spectrum of π-electrons. It is shown that the pulse stably propagates in the medium, taking into account both of these factors. In this case, the magnetic field and tension slow down the pulse, as well as change its amplitude.

**Key words:** localized pulses, gauge theory, magnetic flux, acoustic field, carbon nanotubes.

## Introduction

Extremely short optical pulses of femtosecond duration are of great technological and fundamental interest. They are also the subject of many recent studies of nonlinear optics [2–5].

Such short light pulses have potential applications in the spectroscopy of dielectrics, semiconductors and transient chemical processes, light propagation in the atmosphere and at the interface of materials [1].

Nonlinear optics usually works with almost harmonic electromagnetic waves, modulated by the envelope, under which there are about 100–1 000 oscillations. In contrast, an extremely short pulse usually contain only a few oscillations of the electromagnetic field. Moreover, light bullets are of great interest among such pulses. They are localized in all directions and propagating in a nonlinear medium at a constant speed [6; 7].

It should be noted, that the successes of modern laser technologies in terms of the formation of powerful electromagnetic radiation with given characteristics, including light bullets, are an incentive for a comprehensive study of such pulses in various media, including carbon nanotubes [8]. An important issue is the study of the pulse behavior in a medium under the action of strong external fields. The authors of [9] considered the influence of external strains in the one-dimensional case.

In this paper, we study the dynamics of two-dimensional light bullet in a medium with CNTs at the presence of an acoustic and a constant magnetic field.

## 1. Model and basic equations

The electron spectrum for zig-zag carbon nanotubes $(n, 0)$ in the presence of a magnetic field directed along the CNT axis has the form:

$$\varepsilon(p_z, s) = \gamma\sqrt{1 + 4\cos(ap_y)\cos\left(\frac{\pi}{n}(s + \frac{\Phi}{\Phi_0})\right) + 4\cos^2\left(\frac{\pi}{n}(s + \frac{\Phi}{\Phi_0})\right)}, \tag{1}$$

where $\gamma \approx 2.7$ eV; $a = 3b/2\hbar$; $b = 0,142$ nm is the distance between the adjacent carbon atoms; $(p_y, s)$ is the quasi-momentum, where $p_y$ is the pulse component along the CNT axis; $s = 0, .., n$; $\Phi$ is the magnetic flux through the CNT cross section; $\Phi_0 = \frac{\hbar c}{e}$ is the magnetic flux quantum [10], $e$ is the electron charge, $c$ is the light velocity.

We consider the interaction between carbon nanotubes to be weak. And it is not taken into account here. The electric field $\mathbf{E}$ is directed along the nanotubes axis $(OY)$, and the electromagnetic pulse moves in the transverse direction $(OZ)$.

The acoustic field is taken into account in the framework of the gauge theory and is associated with the appearance of a stress field caused by the strain field. This field is determined by the corresponding vector potential $\mathbf{A}'$, which changes the momentum of electrons in the medium containing the array of carbon nanotubes. In deformed CNTs, all interatomic bonds turn out to be nonequivalent, and the three hopping integrals may not be equal to each other. Since CNTs are a rolled sheet of graphene (the $ZOY$ plane) in the cylinder along the $OY$ axis, we write all the equations for graphene, and then take into account the periodic boundary conditions. In accordance with this, the calibration vector potential has the form: $\mathbf{A}' = (A'_z, A'_y)$, whose components can be written in the form [11]:

$$A'_z = \frac{\sqrt{3}}{2}\,(\gamma_3 = \gamma_2), \qquad A'_y = \frac{1}{2}\,(\gamma_3 + \gamma_2 - 2\gamma_1), \tag{2}$$

where $\gamma_1$, $\gamma_2$, $\gamma_3$ are the hopping integrals.

In the case of weak deformation of the crystal lattice, each hopping integral can be expanded in a series up to the second term [12]:

$$\gamma_i = \gamma + \frac{\beta\gamma}{a^2}\,\mathbf{r}_i\,(\mathbf{u}_i - \mathbf{u}_0), \tag{3}$$

here $\gamma$ is the unperturbed hopping integral; $\mathbf{r}_i$ is the radius vector of nearest neighbors; $\mathbf{u}_i$ is the displacement vector of the $i$-th atom; $u_0$ is the displacement vector of the central atom; $\beta$ is the Grüneisen electronic parameter, which expresses a change in the frequency of lattice vibrations depending on changes in the volume of the system [13]. For carbon structures it is equal 2.

In the continuum limit, one can expand the displacement of carbon atoms:

$$\mathbf{u}_i - \mathbf{u}_0 \propto (\mathbf{r}_i\nabla)\mathbf{u}, \tag{4}$$

$\mathbf{u}$ is the displacement field.

Substituting (3) into (2) taking into account (4), we obtain:

$$A'_z = \chi\,\frac{\beta\gamma}{a}(u_{zz} - u_{yy}), \qquad A'_y = -\chi\,\frac{2\beta\gamma}{a}\,u_{zy}, \tag{5}$$

where $\chi$ is the parameter depending on the characteristics of the chemical bond in the substance, which can be set for CNTs equal to 1 [14].

Thus, the strain gauge field is proportional to the strain tensor $u_{\alpha\beta}$, which determines the local strain of the lattice. By setting the deformation field $\mathbf{u}$, we obtain that the strain tensor in the linear approximation has a well-known form [15]:

$$u_{\alpha\beta} = \frac{\partial_\alpha u_\beta + \partial_\beta u_\alpha}{2}. \tag{6}$$

The calibration potential changes the band structure by calibrating the pulse by $-qA/c$ in the same way as the external electromagnetic field. The contributions of the electromagnetic field and lattice deformations are reduced to the sum of the corresponding vector potentials. The model does not take into account the rotations of interatomic bonds. Based on these assumptions, only one correction $A_z$ is taken into account in the effective equation for the vector potential.

The longitudinal and transverse components of the strain tensor are related by the known relation [15]: $u_{zz} = -\mu u_{yy}$, $\mu = 0,19$ is the Poisson's ratio for CNTs [16].

In the two-dimensional case, the equation describing the propagation of the light bullet in the array of carbon nanotubes takes the form:

$$\begin{gathered}\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial z^2} - \frac{\varepsilon}{c^2}\frac{\partial^2 A}{\partial t^2} - 4\pi j(A + A'/e) = 0,\\ A' = \chi\,\frac{\beta\gamma u_{zz}}{a}\,(1+\mu),\end{gathered} \tag{7}$$

here $\varepsilon$ is the dielectric constant of the medium; the current density $j$ is determined by the formula:

$$j = 2\varepsilon \sum_{s=1}^{n} \int\limits_{BZ} \nu(p_z, s)\cdot f(p_z, s)\,dp, \tag{8}$$

where $\nu(p, s) = \partial\varepsilon(p_y, s)/\partial p_y$ is the electron velocity; $f(p_y, s)$ is the Fermi distribution function; $\varepsilon(p_y, s)$ is determined by the formula (1), integration is carried out in the first Brillouin zone ($BZ$). We omit the calculation of current density in this paper, because it repeats the standard calculations for CNTs, and we present only the final form of the effective equation:

$$\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial z^2} - \frac{\varepsilon}{c^2}\frac{\partial^2 A}{\partial t^2} - \frac{4\pi e n_0 \gamma a}{c}\sum_{q=1}^{\infty} F_q \sin\left(\frac{aq(eA + A')}{c}\right) = 0, \tag{9}$$

where

$$F_q = -q\,\frac{\sum\limits_{s=1}^{n} \frac{b_{sq}}{\gamma} \int\limits_{-\pi}^{\pi} d(p_y\,a)\cdot\cos(q\,a\,p_y)\cdot\exp\left(-\sum\limits_{q=1}^{\infty}\cos(q\,a\,p_y)\cdot b_{sq}/k_B T\right)}{\sum\limits_{s=1}^{n} \int\limits_{-\pi}^{\pi} d(p_y\,a)\cdot\exp\left(-\sum\limits_{q=1}^{\infty}\cos(q\,a\,p_y)\cdot b_{sq}/k_B T\right)};$$

$$b_{sq} = \frac{a}{\pi}\int\limits_{-\pi/a}^{\pi/a} d(p_y\,a)\cdot\varepsilon(p_y, s)\cdot(q\,a\,p_y);$$

$n_0$ is the electron concentration; $k_B$ is the Boltzmann constant; $T$ is the temperature; $b_{sq}$ are the coefficients in the expansion of the electron dispersion law (1) in a Fourier series.

We make the dimensionlessness of the quantities included in the equation (9):

$$\tilde{A} = \frac{eaA}{c},\ \tilde{A}' = \frac{aA'}{c},\ \tilde{x} = \frac{x}{a_0},\ \tilde{z} = \frac{z}{a_0},\ \tilde{t} = \frac{c\cdot t}{a_0},\ a_0 = \frac{c}{2|e|a\sqrt{\pi n_0 \gamma_0}}.$$

The initial condition is chosen in the form:

$$\tilde{A}(\tilde{x}, \tilde{z}, 0) = Q\cdot\exp\left(-\frac{\tilde{x}^2}{l_x^2} - \frac{\tilde{z}^2}{l_z^2}\right),$$

$$\frac{d\tilde{A}(\tilde{x}, \tilde{z}, 0)}{d\tilde{t}} = \frac{2\tilde{z}\,v\,Q}{l_z^2}\cdot\exp\left(-\frac{\tilde{x}^2}{l_x^2} - \frac{\tilde{z}^2}{l_z^2}\right), \tag{10}$$

$$v = \nu_z/c.$$

Where $Q$ is the amplitude of the electromagnetic pulse at the entrance to the environment with CNT; $l_x$, $l_z$ are determined the pulse width along the $x$ and $z$ axis, $\nu_z$ is the pulse velocity along $z$-axis.

Next, numerical simulation is carried out using an explicit second-order finite-difference scheme [17] with zero Neumann boundary conditions for the following system parameters: CNTs of the zig-zag type (7, 0), $\varepsilon = 4$, $n_0 = 10^{24} m^{-3}$, the coefficients $F_q$ determined by equation (9) are calculated at a temperature $T = 77$ K [18], $\nu = 0.9$. The relaxation time in CNTs is $t_{\text{rel}} \approx 10^{-12}$ s, the pulse duration $t_{\text{pulse}} \approx 2\cdot 10^{-15}$ s, thus $t_{\text{pulse}} \ll t_{\text{rel}}$.

The evolution of the electromagnetic pulse is presented in figure 1. We draw the pulse intensity $I$, which can be determined as $I = c^{-2}(\partial A/\partial t)^2$.

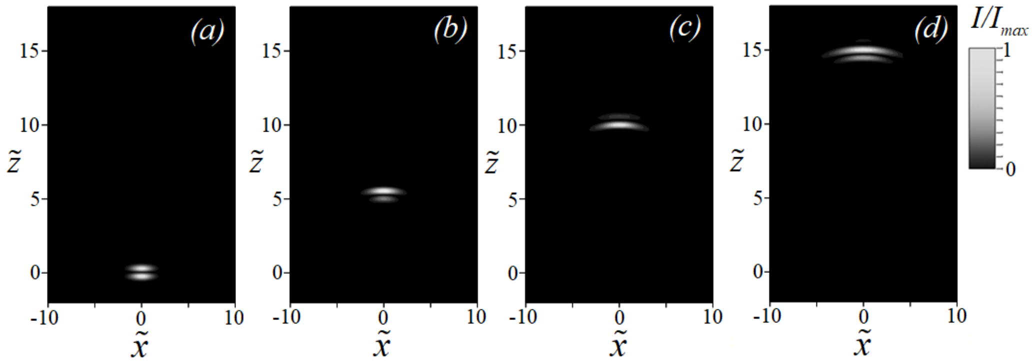


Fig. 1. Evolution of light bullet ($\tilde{u}_{zz} = 0,1$, $\Phi/\Phi_0 = n/2$):
a) $\tilde{t} = 0$; b) $\tilde{t} = 3,5$; c) $\tilde{t} = 6,5$; d) $\tilde{t} = 9,5$.
$I_{\max}$ is the maximum of the intensity for time value $\tilde{t}$

From figure 1 it can be concluded that the light bullet is stable in the CNT array under the influence of acoustic and magnetic fields, since the pulse travels about 10 of its wavelengths. Note that the pulse also exibits a slight diffraction spreading. Let us study the influence of the magnetic field on the light bullet propagation. A two-dimensional view is shown in figure 2, a longitudinal section ($\tilde{x} = 0$) is in figure 3.

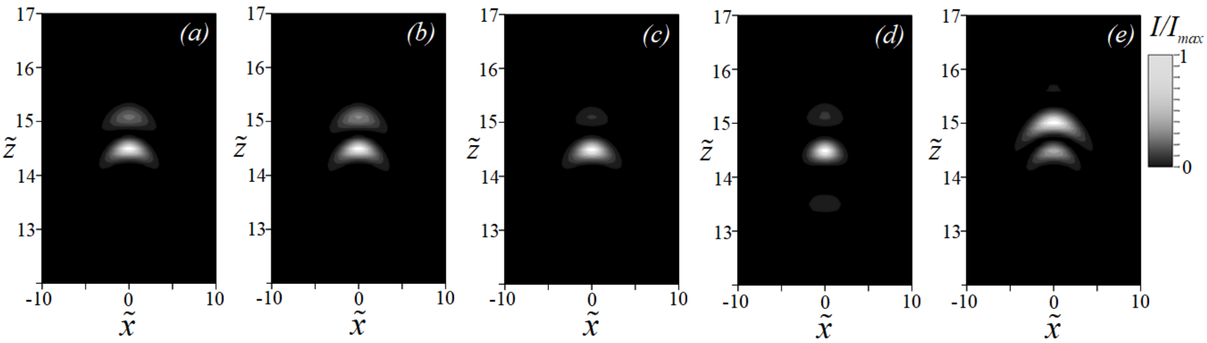


Fig. 2. The intensity of the electric field of the light bullet ($\tilde{t} = 9,5$):
a) $\tilde{u}_{zz} = 0$, $\Phi/\Phi_0 = 0$. Figures (b–e) for $\tilde{u}_{zz} = 0,1$: b) $\Phi/\Phi_0 = 0$;
c) $\Phi/\Phi_0 = n/6$; d) $\Phi/\Phi_0 = n/3$; e) $\Phi/\Phi_0 = n/2$.
$I_{\max}$ is the maximum of the intensity for time value $\tilde{t}$

Figure 2a shows the pulse shape without taking into account the magnetic field and mechanical deformation. Figures 2b–e are plotted in the presence of mechanical tension and for different values of magnetic flux. It cab be seen when the magnetic field increases, the pulse slows down. Also for figure 2d the appearance of a “tail” behind the main pulse is observed as before [8].

The given dependence shows that, controlling the magnitude of the magnetic field, we can change not only the shape, but also the amplitude of the pulse.

The dependence of the intensity of the electric field on the acoustic field magnitude is shown in figure 4.

It can be seen, that in the presence of a magnetic field, but at zero mechanical tension, the pulse retains its localization region, but its amplitude increases. When the tension increases (fig. 3c, d) we observe that the amplitude decreases. Moreover, the larger the value of $\tilde{u}_{zz}$ (fig. 4d), the closer the pulse shape to the initial one (fig. 4a).

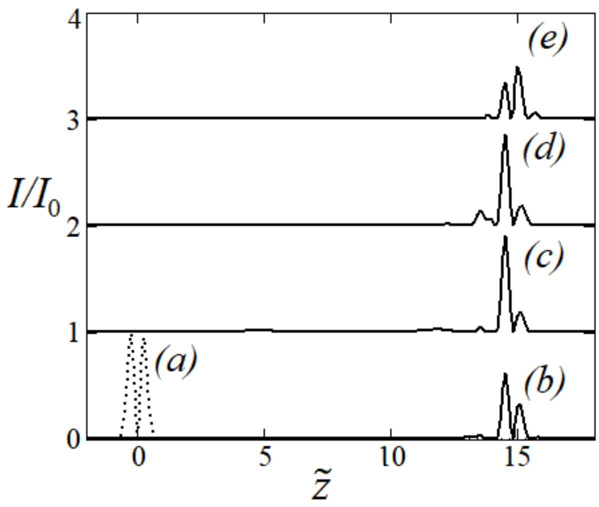


Fig. 3. The intensity of the electric field of the light bullet,
a longitudinal section at $\tilde{x} = 0$ ($\tilde{u}_{zz} = 0,1$): a) pulse at the initial time moment;
Others for $\tilde{t} = 9,5$: b) $\Phi/\Phi_0 = 0$;
c) $\Phi/\Phi_0 = n/6$, for clarity, the curve is raised by 1 unit along the vertical axis;
d) $\Phi/\Phi_0 = n/3$ the curve is raised by 2 units along the vertical axis;
e) $\Phi/\Phi_0 = n/2$ the curve is raised by 3 units along the vertical axis.
$I_0$ is the maximum of the intensity for time value $\tilde{t} = 0$

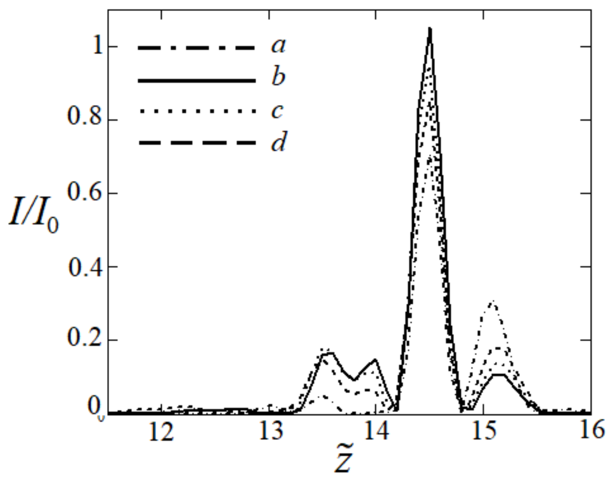


Fig. 4. The intensity of the electric field of the light bullet (a longitudinal section at $\tilde{x} = 0$, $\tilde{t} = 9,5$):
a) $\tilde{u}_{zz} = 0$, $\Phi/\Phi_0 = 0$. Figures (b–d) correspond to $\Phi/\Phi_0 = n/3$:
b) $\tilde{u}_{zz} == 0$; c) $\tilde{u}_{zz} = 0,05$; d) $\tilde{u}_{zz} = 0,1$.
$I_0$ is the maximum of the intensity for time value $\tilde{t} = 0$ at $\tilde{u}_{zz} = 0$ and $\Phi/\Phi_0 = 0$

## Conclusion

Key results of this work are summarized as follows:

1) The numerical modeling showed that the acoustic and magnetic fields significantly affect the dynamics of the light bullet in the carbon nanotubes array.
2) It is observed, that using the magnetic flux, we can change the pulse shape, its region of the localization and the amplitude. Thus, the magnetic field is the controlling parameter for the electromagnetic field of the light bullet.
3) The effect of deformation is manifested both in a change in the shape of the pulse and its amplitude.

## NOTE

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# МОДЕЛИРОВАНИЕ РАСПРОСТРАНЕНИЯ ДВУМЕРНОЙ СВЕТОВОЙ ПУЛИ В МАССИВЕ УГЛЕРОДНЫХ НАНОТРУБОК С УЧЕТОМ МЕХАНИЧЕСКОЙ НАГРУЗКИ И МАГНИТНОГО ПОЛЯ

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**Аннотация.** В данной работе мы исследуем влияние акустического и магнитного полей на процесс распространения локализованного в двух направлениях предельно короткого оптического импульса в среде, содержащей массив полупроводниковых углеродных нанотрубок zig-zag типа. Мы считаем, что расстояние между соседними нанотрубками существенно превышает их диаметр, то есть взаимодействие между углеродными нанотрубками считается слабым и можно им пренебречь. Учет акустического поля проводился в рамках калибровочной теории. Появление этого поля обусловлено появлением поля напряжений, которое вызывается механическими нагрузками на кристаллическую решетку углеродных нанотрубок. Магнитное поле прикладывается вдоль оси нанотрубок и приводит к изменению электронного спектра $\pi$-электронов. Показано, что импульс стабильно распространяется в среде с учетом обоих этих факторов. При этом магнитное поле и деформация приводят к замедлению импульса, а также к изменению его амплитуды. Также наблюдается появление «хвоста» за основным импульсом

**Ключевые слова:** локализованные импульсы, калибровочная инвариантность, магнитный поток, акустическое поле, углеродные нанотрубки.