⁰⁶ Light bullets with Bessel cross section in the environment carbon nanotubes

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The propagation of three-dimensional extremely short optical pulses (light bullets) with a Bessel cross section in a medium of carbon nanotubes placed in an optical resonator is considered. As a result of numerical calculations, it was found that such pulses propagate stably with conservation of energy in a limited region of space, including at large times of the order of 100 ps.

Keywords: extremely short optical pulses, nonlinear medium, light bullets, carbon nanotubes.

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Introduction

Currently nondiffraction optical beams (with transverse cross section of Bessel, Airy and Mathieu), which are pulses spreading without variation of shape and amplitude, are of the substantial interest for non-linear optics. Diffraction diffusion of pulses is a fundamental feature of freely propagating optical beams easily observed in everyday life. As it is known, diffraction considerably impacts the optical resolution limit in various industries, including in microscopy, lithography and photography, as well as at the spectral analysis accuracy limit [1]. Therefore, nondiffraction beams have certain advantages compared to other beams of comparable transverse size, for example, retention of pulse shape widening and scale during its propagation.

This paper will consider Bessel beams. Unique features of these beams are characterized by the fact that the beam may be formed in non-linear environments, the refraction index of which varies weakly on a periodical basis depending on length [2]. Bessel beams may be generated along spiral [3–5], snake- or zigzag-like [6] trajectories. Methods to generate nondiffraction beams of Bessel type that may propagate along random trajectories were proposed in [7] and further observed in [8].

Carbon nanotubes (CNT) were chosen as pulse propagation medium, as having unique physical properties in the optical range because of nonparabolicity of the electron dispersion law [9,10]. Simplicity of their structure, uniqueness of properties [11-15] promote research in the field of optical pulses propagation, design of optical devices on their basis, but the main property that CNTs have the ability of using them as a medium to form light bullets [16–19]. Carbon nanotubes are of the utmost interest for many researchers. They have become widely popular in non-linear optics, and thanks to that play one of key roles in design of various optics, nanophotonics etc. devices. The objective of propagation of pulses with various shapes in non-linear medium is not a trivial one. A textbook case is a "theorem of areas" in a unidimensional problem on self-induced transparency. Thus, pulses with "area" of more than 2π , are resistant, and pulses of smaller area decompose in a dispersion manner. Pulse area is an integral of Rabi frequency by time within the limits of $t = -\infty$ (when the pulse did not exist) to a certain rather long time t (when the pulse has already passed by) [20]. It is evident that in case of Bessel pulses that propagate consistently in the linear medium through interference of diffraction waves from the side tabs, their dynamics in the non-linear medium is another problem. Carbon nanotubes were chosen as an object where non-linear response of the medium may be calculated analytically with any preset accuracy.

In this paper CNTs form a heterogeneous medium placed into an optical resonator. The resonator applies intraresonator laser spectroscopy, and multiple reflection of the pulse from its walls causes pulse energy losses because of diffraction [21]. It should also be noted additionally that effects arise that are related to reflection from cylindrical resonator walls. The beam passes through the CNT array many times owing to multiple reflection from the cylindrical resonator walls. The important advantage of such pulses (resonator soliton waves) is the fact that they may propagate, having optical feedback, even when in absence of the resonator the same non-linear medium does not support any spatial soliton waves.

Previously the authors already conducted research dedicated to propagation of shortest optical pulses, including of Bessel cross section, in the CNT media [22–25], however, this paper will be first to numerically simulate dynamics of pulses at longer periods of time (to 140 ps), which is critical for applied problems. Another distinctive feature of the paper is the fact that heterogeneous CNT medium is placed under the conditions of the optical resonator. Therefore, the problem on propagation of nondiffraction pulse with Bessel cross section in the medium of ordered CNTs placed into an optical resonator plays an important role both from theoretical and applied points of view.

Main equations

This paper will consider the following approximations: pulse-induced charge along axis of carbon nanotubes, and electric field of the substrate are not taken into account. The specific distance between nanotubes and their size is many times smaller than the size of the spatial area, where the Bessel optical beam is localized. This makes it possible to consider the current spread in the volume and to apply the continuous medium approximation.

The proposed system is simulated so that the 3D shortest optical pulse propagates in the heterogeneous medium of CTN such as zig-zag in the optical resonator, electric field of which is directed along the axis of nanotubes (fig. 1).

The Hamiltonian of the electron system has the appearance of

$$H = \gamma \sum_{j\sigma} a_{j\sigma}^* a_{j\sigma} + c.c., \qquad (1)$$

where $a_{j\sigma}^+$, $a_{j+\Delta\sigma}^-$ operators of electron creation and destruction at node *j*.

Let us write Fourier transform that diagonalizes the Hamiltonian *H*:

$$a_{n\sigma}^{+} = \frac{1}{\sqrt{N^{1/2}}} \sum_{j} a_{j\sigma}^{+} \exp(ijn),$$
$$a_{n\sigma} = \frac{1}{\sqrt{N^{1/2}}} \sum_{j} a_{j\sigma} \exp(-ijn).$$
(2)

Spectrum of electrons describing the properties of the electronic subsystem in absence of Coulomb repulsion of CNT type "zig-zag" has the appearance of [26]

$$\varepsilon_{s}(p) = \pm \gamma \left\{ 1 + 4\cos(ap)\cos\left(\pi \frac{s}{m}\right) + 4\cos^{2}\left(\pi \frac{s}{m}\right) \right\}^{1/2},$$
(3)



Figure 1. Geometry of the problem. Current and electric field of the pulse are directed along CNT axis.

where s = 1, 2...m, nanotube type is (m, 0), $\gamma \approx 2.7 \text{ eV}$, $a = 3b/2\hbar$, b = 0.142 nm — distance between adjacent carbon atoms, p — quasipulse.

Maxwell's equations describing the energy of shortest optical pulse with Bessel cross section may be written as follows [2,27]:

$$\frac{\partial^{2}\mathbf{E}}{\partial x^{2}} + \frac{\partial^{2}\mathbf{E}}{\partial y^{2}} + \frac{\partial^{2}\mathbf{E}}{\partial z^{2}} - \frac{1}{c^{2}}\frac{\partial^{2}\mathbf{E}}{\partial t^{2}} + \frac{4\pi}{c}\frac{\partial\mathbf{j}}{\partial t} + \frac{4\pi}{c^{2}}\frac{\partial^{2}\mathbf{P}}{\partial t^{2}} = 0,$$
(4)

where **j** — electric current density, c — light speed in the medium, t — time, **E** — electric field of light bullet, **P** = μ **E**, where **P** — polarization vector parallel to vector of electric field of the pulse **E**, μ — coefficient of linear susceptibility.

We modify equation (4), taking into account Coulomb calibration to describe propagation of pulses with wide spectrum in non-linear medium:

$$\mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}.$$
 (5)

Having integrated equation (4) by time, we obtain the generalized equation for vector-potential **A** for a non-linear medium:

$$\frac{\partial^2 \mathbf{A}}{\partial x^2} + \frac{\partial^2 \mathbf{A}}{\partial y^2} + \frac{\partial^2 \mathbf{A}}{\partial z^2} - \frac{1}{c^2} \left(1 + 4\pi\mu\right) \frac{\partial^2 \mathbf{A}}{\partial t^2} + \frac{4\pi}{c} \mathbf{j} = \mathbf{0}.$$
 (6)

Vector-potential **A** has the appearance of: A(0, A(r, z, t), 0), and current density -j(0, j(r, z, t), 0). Let us write a standard equation for current density in the form of

$$\mathbf{j} = en(z, r) \sum_{ps} v_s \left(\mathbf{p} - \frac{e}{c} \mathbf{A}(t) \right) \langle a_{ps}^+ a_{ps} \rangle, \qquad (7)$$

where $v_z = \frac{\partial \varepsilon_s(\mathbf{p})}{\partial \mathbf{p}}$, brackets mean averaging with nonequilibrium matrix of density $\rho(t)$: $\langle B \rangle = Sp(B(0)\rho(t))$. Taking into account the fact that $[a_{ps}^+ a_{ps}, H] = 0$, from motion equations for density matrix we immediately get that $\langle a_{ps}^+ a_{ps} \rangle = \langle a_{ps}^+ a_{ps} \rangle_0$, where $\langle B \rangle_0 = Sp(B(0)\rho(t))$, n(z, r) — CNT density [28].

With account of the fact that $\rho_0 = \frac{\exp\{-H/k_B T\}}{S_P(\langle B \rangle = S_P(B(0)\rho(t)))}$, where k_B — Boltzman's constant, T — temperature, let us expand $v_s(\mathbf{p})$ into Fourier series, and we obtain

$$v_{s}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}(t)\right) = \sum_{k} A_{ks}\left(\sin(k\mathbf{p})\cos\left(\frac{ke}{c}\mathbf{A}(t)\right) - \cos(kp)\sin\left(\frac{ke}{c}\mathbf{A}(t)\right)\right), \quad (8)$$

where $A_{ks} = \int_{-\pi/a}^{\pi/a} = v_s(\mathbf{p})\sin(k\mathbf{p})d\mathbf{p}$ — serial expansion coefficients that diminish with growth of k.



Figure 2. Dynamics of light bullet with Bessel cross section in heterogeneous medium (lattice constant $\chi = 0.5 \,\mu$ m) for CNTs placed in the optical resonator at time moments t = 10 (*a*), 20 (*b*), 40 (*c*), 60 (*d*), 80 (*e*), 100 (*f*), 120 (*j*), 140 ps (*h*).

If you take into account the fact that distribution function ρ_0 — even function of quasipulse **p**, which gives zero when averaged with $\sin(k\mathbf{p})$, equation (8) may be presented as

$$v_s\left(\mathbf{p} - \frac{e}{c}\mathbf{A}(t)\right) = -\sum_k A_{ks}\cos(k\mathbf{p})\sin\left(\frac{ke}{c}\mathbf{A}(t)\right).$$
 (9)

Substituting this equation in (7) and summing up by p and s, we obtain

$$\mathbf{j} = -en_0 \sum_k B_k \sin\left(\frac{ke}{c} \mathbf{A}(t)\right),$$
$$B_k = \sum_{s=1-\pi_{-\pi/a}}^{\pi/a} \int_{-\pi/a}^{\pi/a} A_{ks} \cos(k\mathbf{p}) \frac{\exp\{-\beta\varepsilon_s(\mathbf{p})\}}{1 + \exp\{-\beta\varepsilon_s(\mathbf{p})\}}, \quad (10)$$

where n_0 — concentration of equilibrium electrons in carbon nanotubes, $\beta = 1/k_BT$.

If you take into account all the above, equation (6) in cylindrically symmetrical case after transition to nondimensional values will have the appearance of

$$\frac{\partial^2 \widetilde{\mathbf{A}}}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \widetilde{\mathbf{A}}}{\partial r} \right) - \frac{1}{c^2} \frac{\partial^2 \widetilde{\mathbf{A}}}{\partial t^2} + \frac{4\pi}{c} n(z, r) \widetilde{\mathbf{j}} = 0,$$
(11)

where $r = \sqrt{x^2 + y^2}$, the member of sum depending on the angle of turn tends toward zero, $\widetilde{\mathbf{A}}$ — nondimensional vector-potential, $\widetilde{\mathbf{j}}$ — nondimensional current density. Further in our calculations coefficient n(z, r) will be set as $n(z, r) = 1 + a \cos(2\pi z/\chi)$, where *a* sets the non-linearity

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Figure 3. Integral intensity by cross cut of the resonator at various moments of time t = 10 (*a*), 20 (*b*), 40 (*c*), 60 (*d*), 80 (*e*), 100 (*f*), 120 (*j*), 140 ps (*h*).

modulation depth, χ — modulation period. The paper considers the modulation along axis z. The optical resonator is presented in cylindrical form and is simulated by setting periodical boundary conditions along the cylinder axis and by introduction of boundary conditions of reflection at the cylinder boundary. Notice that equation (11) is a generalization of a well-known Sine-Gordon equation.

Research results

Initial conditions for vector-potential of pulse electric field were set as follows:

$$\mathbf{A}(z,r) = Q \exp\left\{-\frac{(z-z_0)^2}{\gamma_z^2}\right\} J_0\left\{\left|\frac{(r-r_0)}{\gamma_r}\right|\right\}$$
$$\times \exp\{-\Delta|r-r_0|\},$$
$$\frac{d\mathbf{A}(z,r)}{dt} = \frac{2\upsilon z Q}{\gamma_z^2} \exp\left\{-\frac{(z-z_0)^2}{\gamma_z^2}\right\} J_0\left\{\left|\frac{(r-r_0)}{\gamma_r}\right|\right\}$$
$$\times \exp\{-\Delta|r-r_0|\}.$$

Here Q — pulse amplitude, Δ — cutting parameter, which is introduced since the beam with Bessel cross section may not be physically realized, and the function must be cut at large distances to produce the finite energy of the beam, γ_z , γ_r — pulse width in directions z and r, v — initial speed of the pulse.

As results of the numerical calculations shown in fig. 2 demonstrated, propagation of 3D light bullet with Bessel cross section in the medium of ordered CNTs placed in the optical resonator is quasi-resistant and quasi-stable, i.e. energy of electromagnet pulse remains localized in the limited spatial area.

Electric field intensity is expressed in relative units and proportionate to electric field square:

$$I(\text{arb. units}) \propto E^2 = \left(E \cdot \frac{\omega_0}{c}\right)^2$$

 $\omega_0 = 2|e|d_x h^{-1} \sqrt{\pi \gamma_0 n}.$

Notice that all values in the expression above are measured in SI system. From the dependencies given it is seen that



Figure 4. Integral intensity near axis of the cylindrical resonator at moments of time t = 10 (*a*), 20 (*b*), 40 (*c*), 60 (*d*), 80 (*e*), 100 (*f*), 120 (*j*), 140 ps (*h*).

light bullets with Bessel cross section in heterogeneous CNT medium under conditions of the optical resonator propagate as quasi-resistant, however, the pulse shape is still subject to dispersion diffusion. Shape change is clearly demonstrated in fig. 3 and 4. Thus, fig. 3 shows cuts of integrals along the entire cross section of the resonator from intensity, while fig. 4 shows integrals by intensity in the cross section near the integration axis.

Values of the corresponding Poynting?s vector are shown in fig. 5, which illustrates expansion of the pulse along the radial direction (in direction towards the resonator walls) and subsequent return of the pulse energy back to the resonator axis.

As seen from the provided figures, electric field of the bullet in large times remains concentrated along the axis of the cylindrical resonator, and in this sense we may talk about quasi-stable propagation of a light bullet.

Impact of the non-linearity modulation depth α manifests itself in minor change of the shortest pulse shape. Modulation period χ significantly impacts pulse speed, — as the period reduces, the pulse reflects more frequently from the non-linear medium nodes, accordingly, interference of the straight and reflected waves is more frequent, therefore, the pulse speed drops. It is evident that infinite period (absence of interference) will maximize the pulse speed. This result was confirmed many times for pulses of femtosecond duration in media with oriented CNTs [22,23].

Light bullet amplitude varies with time as seen in fig. 2–4. It should be noted that amplitude value varies insignificantly, within several relative units. Notice that such behavior, namely pulse shape variation, is related to both transverse structure of the pulse (internal oscillatory modes of the pulse are excited) and to the heterogeneity of the medium (the medium refraction index has spatial modulation). Therefore, the Bessel structure will not be fully maintained. Nevertheless, energy localization occurs at the expense of the multiple reflection of waves from resonator walls and subsequent interference.

Summing up, it may be said that this paper was first to numerically model the dynamics of shortest optical pulses with Bessel cross section in the heterogeneous medium of CNTs placed into the optical resonator. As opposed to



Figure 5. Poynting?s vector components along axis r in the medium of ordered CNTs in the optical resonator at various moments of time t = 30 (a), 40 (b), 60 (c), 80 (d), 100 (e), 120 (j), 140 ps (h).

previously known results, modelling was done on large times, around 140 ps, this is the time that the pulse manages to pass through several dispersion waves (impact of dispersion at pulse duration $L_D = T_0^2/|d^2\beta/d\omega^2|$, where T_0 — initial duration of the pulse), and the second derivative is responsible for the dispersion value, therefore, quasistable propagation of a light bullet may be mentioned, whose energy remains localized in the limited spatial area.

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Conflict of interest

The authors declare that they have no conflict of interest.

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