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Three-dimensional light bullets in a Bragg medium with carbon nanotubes

Alexander V. Zhukov[1] · Roland Bouffanais[1] · Mikhail B. Belonenko[2,3] ·
Ilya S. Dvuzhilov[3] · Yulia V. Nevzorova[3]

Abstract We present a theoretical study of the propagation of three-dimensional extremely short electromagnetic pulses (a.k.a. light bullets) through a Bragg medium containing an immersed array of carbon nanotubes. We demonstrate the possible stable propagation of such light bullets. In particular, our results suggest these light bullets can carry information about the Bragg medium itself.

1 Introduction

Among the vast breadth of nonlinear optical phenomena, the propagation of extremely short three-dimensional (3D) spatiotemporal optical solitons has attracted considerable attention given the range of different properties observed with various nonlinear media [1–6]. Localized electromagnetic wave packet inevitably spreads both in space and time under the concurrent effects of dispersion and diffraction present in any medium. Significant research activity has been dedicated to devising new ways to overcome these universal broadening effects to generate sustained localized wave packets [1–6]. Such traveling wave packets that are localized while retaining their spatiotemporal shape—in spite of diffraction and dispersion effects—are referred to as "light bullets". When propagating through a nonlinear medium, three-dimensional (3D) light bullets tend to

vanish as a consequence of a host of instabilities [3]. One can say that a light bullet is a natural generalization of well-known one-dimensional (1D) electromagnetic solitons [7] to the greater dimension case. In particular, the distinguishing feature of these extremely short pulses—interesting and relevant from several viewpoints, including the technological one—is that it is impossible to make a partition of the form of the electromagnetic pulse between its envelope and its carrier part. As a result, the well-established method of multiscale expansion is no longer suitable for solving Maxwell's equations. The latter must be solved without discarding any derivatives [8, 9]. Note that in general, the medium produces unavoidable dispersive effects. Therefore, the appearance of solutions with localized energy requires consideration of nonlinear effects even in the one-dimensional case.

Nanoscale carbon materials such as carbon nanotubes (CNTs) have strongly pronounced nonlinear properties in the optical range, which make them very attractive for a vast range of uses in applications [10–12]. They can also be used as the medium in which the formation of light bullets occur. Corresponding calculations were made for one-, two- and three-dimensional cases [13–20] and it was found that the CNT medium allows for the possible stable propagation of light bullets. There is only one rather weighty constraint that comes from practical considerations: the speed of propagation of light bullets is only defined by the refractive index of the medium and it can only be tuned in a fairly narrow interval of values. One possible solution to this issue is to consider the additional modulation of the refractive index of the medium, forming the so-called Bragg environment. These considerations were first successfully applied to a two-dimensional case in Ref. [21], while here we address the more challenging and realistic problem associated with the 3D case.

✉ Alexander V. Zhukov
  alex.zhukov@outlook.sg

[1] Singapore University of Technology and Design, 8 Somapah Road, 487372 Singapore, Singapore

[2] Laboratory of Nanotechnology, Volgograd Institute of Business, 400048 Volgograd, Russia

[3] Volgograd State University, 400062 Volgograd, Russia

In the case of a Bragg environment, the propagation speed of the wave packet is defined by both the period and depth of modulation of the refractive index, due to partial reflection and the further interference of the wave packet. In this case, it is theoretically possible to control the speed of light bullets in such an environment. In practice, the refractive index modulation is possible with the use of an external DC field in any environment that allows for either Kerr or Faraday effects, and which contains CNTs. It is worth adding that the light bullets have recently been reported in pure Kerr media [22, 23]. Note that the simple considerations given in Ref. [14] to the existence of light bullet do not apply in the present case owing to the fact that there is no translational invariance. It is also quite obvious that the additional variance introduced by the Bragg environment will not lead to the collapse of the light bullets. The importance of practical applications and the considerations set out above provide the impetus for the present study.

2 Fundamental equations

In our study, we use the strong-coupling approximation for the electronic structure of CNTs in the framework of the analysis of the dynamics of π-electrons. The dispersion relation for a zigzag-type CNT $(m, 0)$ reads as [11]:

$$E_s(\mathbf{p}) = \pm\gamma \left\{ 1 + 4\cos(ap_z)\cos(\pi s/m) + 4\cos^2(\pi s/m) \right\}^{1/2}, \quad (1)$$

where $\gamma = 2.7$ eV, $a = 3b/2\hbar$, and $b = 0.152$ nm is the distance between neighboring carbon atoms. Note that the quasimomentum $\mathbf{p}$ is represented here as $(p_z, s), s = 1, 2, \ldots m$.

The system consists of an ordered array of CNTs embedded into any medium whose refractive index is harmonic along the bullet propagation axis. The variations of the refractive index of this medium are fully characterized by their period and magnitude. When constructing a model of the ultrashort optical pulse propagation in a Bragg environment with nanotube system, where the geometry is shown in Fig. 1, we will describe the electromagnetic pulse field on the basis of Maxwell's equations in the Coulomb gauge [24], namely $\mathbf{E} = -\partial\mathbf{A}/c\partial t$.

The vector-potential is thereby expected to take the reduced form $\mathbf{A} = (0, 0, A_z(x, y, z, t))$. The governing propagation equation can be written as:

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

where $n(x)$ represents the spatial variations of the refractive index along the x-axis, i.e., the 1D Bragg grating; $\mathbf{j}$ is the current density that originates from the influence of the electric field pulse onto the electrons in the conduction band of the CNTs. Here, we neglect the diffraction spreading of the laser beam in the direction along the axis of the nanotubes. The electric field eventually induced by the substrate itself is not considered in this proposed formalism. We also discard possible inter-gap jumps, which results in restricting the possible frequencies of laser pulses to the near-infrared region. The typical size of CNTs and the distance between them are both much smaller than the spatial scale of the region where ultrashort pulses are localized. This means that we can appropriately work under the continuous-medium approximation, and thus consider the current density as homogeneously distributed over a given volume. The characteristic length scale associated with spatial variations of the refractive index in the Bragg medium is even larger, and, therefore, does introduce any further restriction to our modeling framework.

Fig. 1 Geometry of the problem with carbon nanotubes aligned along the z-direction and contributing to generating a Bragg grating along the x-direction
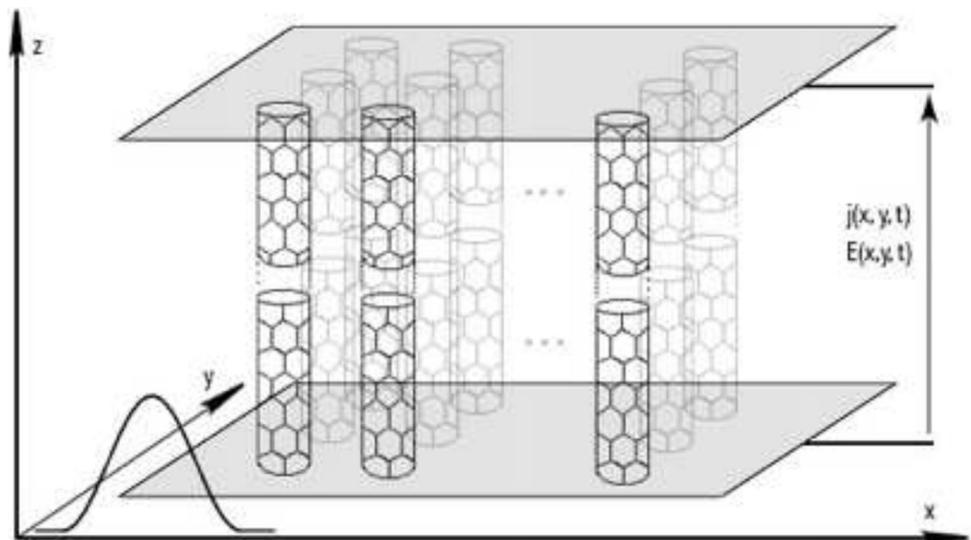
Analytical evaluation of the current density **j** is essentially similar to that provided in Ref. [21]. We, however, provide it here briefly for the sake of self-consistency. Typical relaxation time for electrons in CNTs can be estimated at 3×10^{-13} s, then the electron ensemble (on time scales of the order of 10^{-14} s, which is typical for ultrashort EM pulses) can be described by the collision-less Boltzmann equation:

$$\frac{\partial f_s}{\partial t} - \frac{q}{c} \frac{\partial A_z}{\partial t} \frac{\partial f_s}{\partial p_z} = 0, \tag{3}$$

where $f_s = f(p_z, s, t)$ is the electron distribution function, which implicitly depends on the spatial coordinates; q is the electron charge, and c is the speed of light in vacuum. At the initial instant, the distribution f is classically given by the equilibrium Fermi–Dirac distribution:

$$f_{s0} = \{1 + \exp(E_s(\mathbf{p})/k_B T)\}^{-1},$$

where T is the temperature, and k_B is the Boltzmann constant. The current density $\mathbf{j} = (0, 0, j_z)$ is given by

$$j_z = \frac{q}{\pi \hbar} \sum_s \int f_s(p_z) v_z \, dp_z, \tag{4}$$

where we have introduced the group velocity $v_{sz} = \partial E_s(\mathbf{p})/\partial p_z$. Solving Eq. (3) by means of the method of characteristics allows us to obtain:

$$j_z = \frac{q}{\pi \hbar} \sum_s \int_{-q_0}^{q_0} dp_z v_{sz}\left(p - \frac{q}{c} A_z\right) f_0(\mathbf{p}). \tag{5}$$

The integration in Eq. (5) is performed over the first Brillouin zone with $q_0 = 2\pi \hbar/3b$. The group velocity can conveniently be expanded as a Fourier series:

$$v_{sz}(x) = \sum_m a_{ms} \sin(mx),$$

where

$$a_{ms} = \frac{1}{\pi} \int_{-\pi}^{\pi} v_{sz}(x) \sin(mx) \, dx.$$

The propagation equation for the vector potential becomes

$$\frac{\partial^2 A_z}{\partial x^2} + \frac{\partial^2 A_z}{\partial y^2} + \frac{\partial^2 A_z}{\partial z^2} - \frac{n^2(x)}{c^2} \frac{\partial^2 A_z}{\partial t^2} + \frac{q}{\pi \hbar} \sum_m c_m \sin\left(\frac{maq}{c} A_z\right) = 0, \tag{6}$$

where

$$c_m = \sum_m a_{ms} b_{ms}, \quad \text{with} \quad b_{ms} = \int_{-q_0}^{q_0} dp_z \cos(map_z) f_0(\mathbf{p}).$$

At this stage, for computational convenience, we pass to the cylindrical coordinates, where Eq. (6) reads

$$\frac{\partial^2 A_z}{\partial x^2} + \frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\partial A_z}{\partial r}\right) - \frac{n^2(x)}{c^2} \frac{\partial^2 A_z}{\partial t^2} + \frac{q}{\pi \hbar} \sum_m c_m \sin\left(\frac{maq}{c} A_z\right) = 0, \tag{7}$$

where $r = \sqrt{y^2 + z^2}$.

Our estimations show that the coefficients c_m decrease with increasing m approximately as $(1/2)^m$. Then—when computing Eq. (6)—we can restrict ourselves to the first ten terms, and subsequently increase the number of terms depending on the required accuracy.

3 Results and discussion

For the numerical solution of Eq. (7), we have implemented an explicit finite-difference scheme for hyperbolic equations [30]. The step sizes, both in time and space, were iteratively decreased by a factor of two, until the obtained solution became unchanged to the eighth decimal place. Initial conditions for the vector potential have been chosen to have the following form:

$$A_z(x, r, t = 0) = A_0 \exp\left\{-\frac{x^2}{\gamma^2}\right\} \exp\left\{-\frac{r^2}{\beta^2}\right\}, \tag{8}$$

$$\frac{dA_z}{dt}\bigg|_{t=0} = \frac{2vx}{\gamma^2} A_0 \exp\left\{-\frac{x^2}{\gamma^2}\right\} \exp\left\{-\frac{r^2}{\beta^2}\right\}, \tag{9}$$

where v is the initial pulse velocity, β and γ are the parameters determining the pulse width along r and x, respectively. The refractive index of the medium has been modeled as $n(x) = n_0(1 + \alpha(2\pi x/\chi))$, where α is the modulation depth, and χ is the period of the Bragg grating, where we have taken $\alpha = 0.05$.

The results of numerical calculations show that the propagation of the light bullet is stable and the resulting evolution is shown in Fig. 2.

As can be seen from the resulting dependencies, the light bullet in a Bragg environment with cross-modulation of the refractive index is not experiencing any considerable broadening, but there are energy fluctuations in the environment 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), resulting thereby in a light bullet shape changes. We also note that, despite the change in the shape of the light bullet, its energy is still concentrated in a limited area.
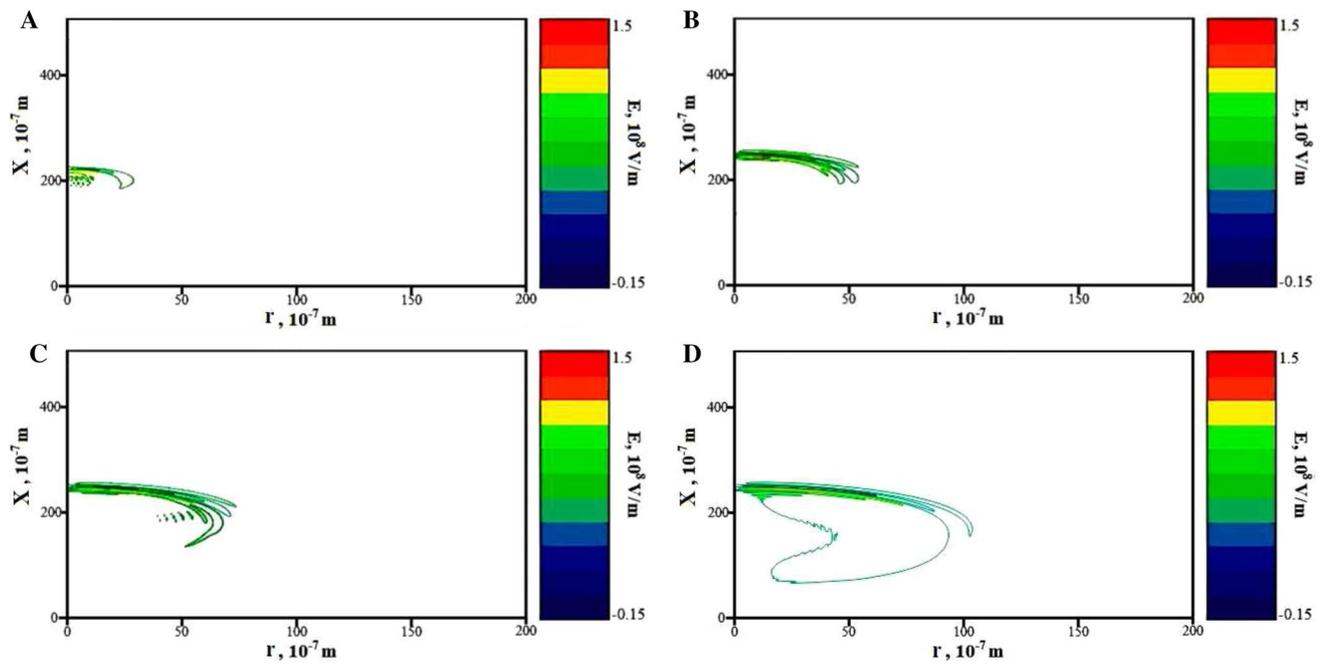
Fig. 2 Propagation of a light bullet in the Bragg environment (lattice period $\chi = 2.5$ μm) with carbon nanotubes at given instants of time ($T_0 = 2.5$ ps): **a** $T = T_0$; **b** $T = 2T_0$; **c** $T = 3T_0$; **d** $T = 4T_0$. Values of the field intensity are mapped on a *color scale*, where the maximum values correspond to *red* and the minimum ones to *dark blue*
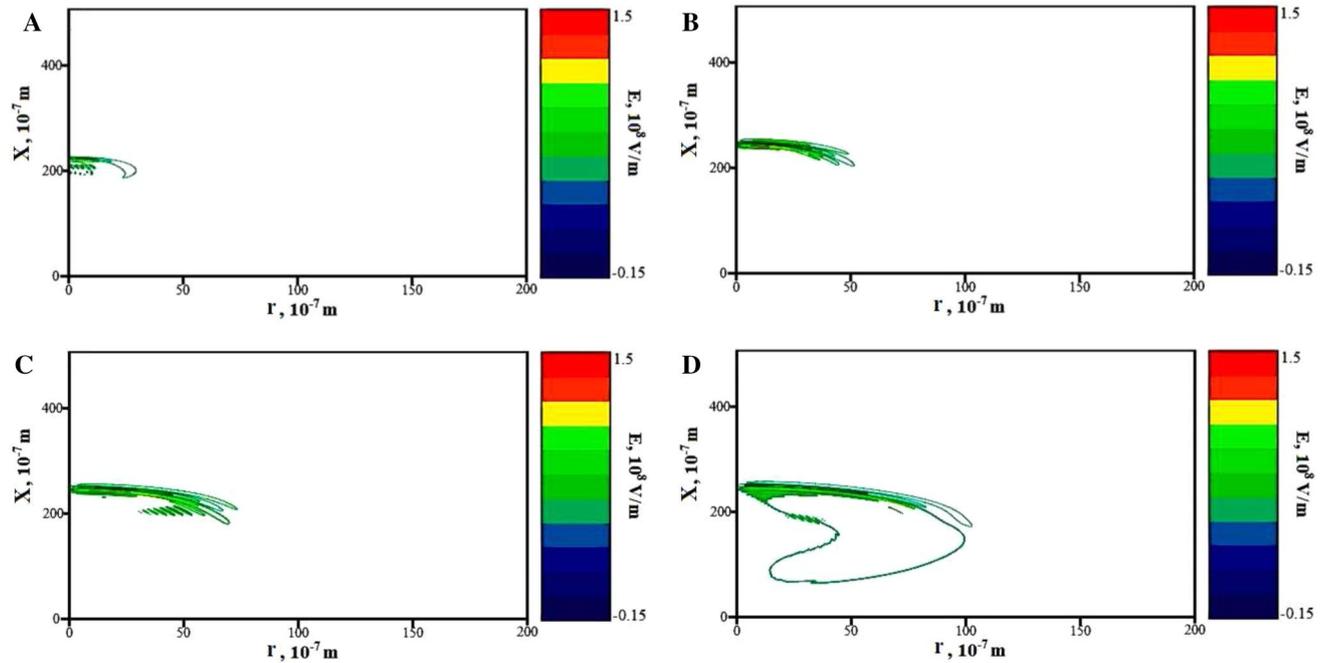

Fig. 3 Propagation of a light bullet in the Bragg environment (lattice period $\chi = 5$ μm) with carbon nanotubes at given instants of time ($T_0 = 2.5$ ps): **a** $T = T_0$; **b** $T = 2T_0$; **c** $T = 3T_0$; **d** $T = 4T_0$. Values of the field intensity are mapped on a *color scale*, where the maximum values correspond to *red* and the minimum ones to *dark blue*

To support our qualitative conclusions, we have performed the same numerical analysis for two and four times larger Bragg periods χ, illustrated in Figs. 3 and 4, respectively.
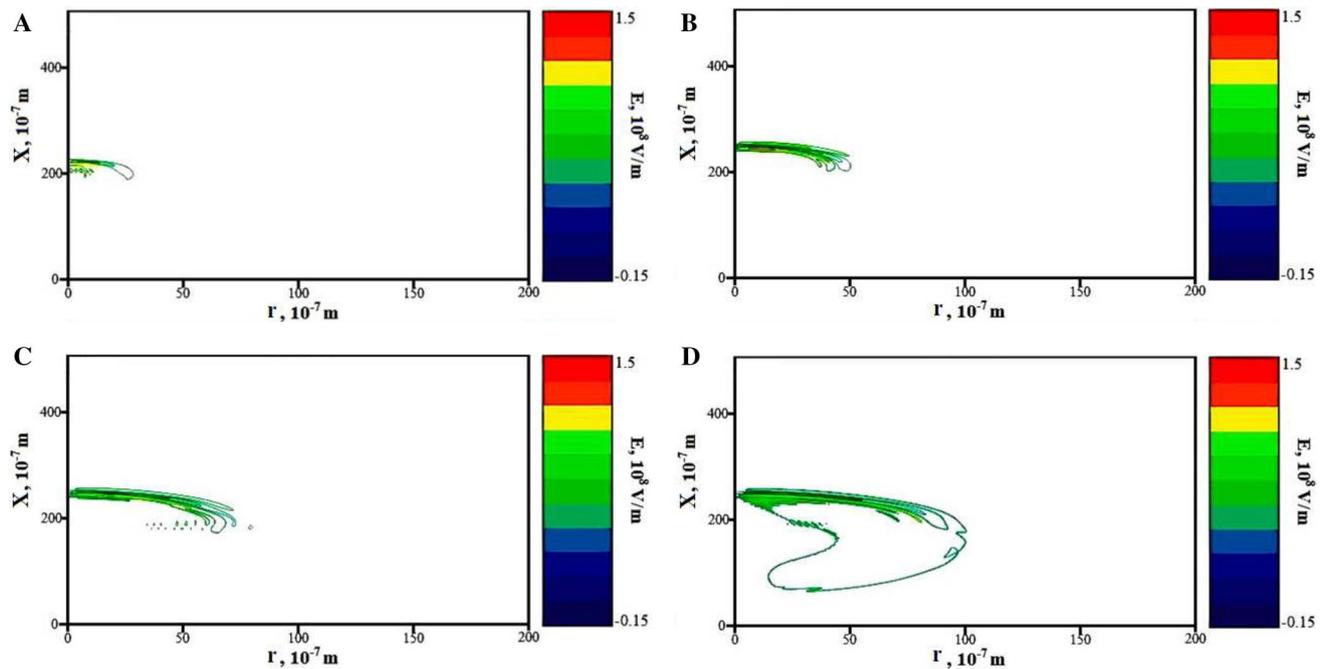
Fig. 4 Propagation of a light bullet in the Bragg environment (lattice period $\chi = 10\ \mu$m) with carbon nanotubes at given instants of time ($T_0 = 2.5$ ps): **a** $T = T_0$; **b** $T = 2T_0$; **c** $T = 3T_0$; **d** $T = 4T_0$. Values of the field intensity are mapped on a *color scale*, where the maximum values correspond to *red* and the minimum ones to *dark blue*

As can be seen from the evolution of the propagation of three-dimensional extremely short optical pulses (Figs. 2, 3, 4), the light bullet somewhat changes its configuration and spreading of shape inevitably occurs over time due to the unavoidable dispersive effects of the medium. By extremely short pulses, we refer to light bullets with spatial extent of the order of 10^{-5} m and temporal duration of the order of 10^{-13} s. These pulses correspond to a few electric field oscillations (less than 10). The solution for three-dimensional light bullets in Bragg environment with carbon nanotubes remains localized, but changes its spatial structure due to the lateral dispersion. The combined effect of the pulse spreading due to the dispersion and nonlinearity leads to the formation of a multi-peak transverse structure, which nevertheless remains localized in a bounded spatial domain.

Thus, we demonstrated the possibility for the stable propagation of three-dimensional light bullets through an array of CNTs immersed in a medium with periodically varying refractive index. Note that from a practical point of view, this result is important because it allows one to control the speed of light bullets by varying the parameters of the Bragg medium—the Bragg period χ. At the same time, the propagation of light bullets in a Bragg medium has some significant differences from the case of a medium with a constant refractive index. Perhaps the most important difference is that the light bullets in a Bragg environment have a more complex transverse structure, which we believe is related to the excitation of internal modes of light bullets resulting from the interaction with the inhomogeneity of the refractive index of the medium. Previously, such an effect has already been observed in the solution of the problem of the interaction of ultrashort pulses with metallic heterogeneity in environments with CNTs [31].

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