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Two-dimensional extremely short electromagnetic pulses in a Bragg medium with carbon nanotubes

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Abstract. We present a theoretical study of the propagation of extremely short electromagnetic pulses in a Bragg medium containing an immersed array of carbon nanotubes. With this unique configuration, we establish 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

The concept of multidimensional solitons that are localized in both space and time, also known as "light bullets", was introduced in pioneering works [1,2], and has since then been investigated in various nonlinear optical media, with emphasis on the specific issue of the stability of solitons [3]. This emerging field of research has led to numerous interesting developments (see, e.g., Refs. [4,5]). One can say that the concept of light bullets is a natural generalization of well-known one-dimensional electromagnetic solitons [6] to cases of higher dimensions. It is worth adding that by the very nature of light bullets, all the energy is concentrated in a finite and bounded region of space.

In addition to its intrinsic scientific interest, the study of spatiotemporal solitary electromagnetic waves should open new avenues for the development of powerful optical information-processing systems. Specifically, in the case of ultrashort pulses, the determining factor is the fact that the electromagnetic pulse shape cannot be classically decomposed into an envelope and a carrier. This leads to the fact that the governing Maxwell's equations cannot be solved by the well-established method of multiscale expansions, and thus one needs to solve them without discarding any derivatives [7,8]. Note that in the case of an optical medium characterized by a given dispersion law – either normal or anomalous, the occurrence of highly-localized energy solutions requires the consideration of nonlinear effects, even in the one-dimensional case. Widely used in applications, carbon nanotubes (CNTs) are considered as one of the most promising building blocks in modern nanoelectronics [9–13]. Among their very many peculiar features, the nonlinearity of the electron dispersion in nanotubes leads to a wide range of properties, which could be used to design a medium enabling the propagation of light bullets. This problem has attracted significant attention in the one-, two- and three-dimensional cases [14–21], leading to a confirmation of the possible propagation of light bullets in environments with CNTs. A thorough and comprehensive review of recent progress in this field can be found in reference [22].

The above studies, however, have dealt with systems where the speed of propagation of light bullets is determined solely by the refractive index of the medium and thus cannot be changed in a fairly wide range. The solution to this kind of problem is well known: it requires modulating the refractive index in one way or another so as to form a so-called Bragg grating environment. In this case, the speed of propagation of a wave packet – due to its partial reflection and interference – is thereby governed by both the period and amplitude of the refractive index modulation. In practice, the refractive index modulation is possible with the use of an external DC field in an any environment that allows for either Kerr or Faraday effects, and which contains CNTs.

Note that the simple considerations reported in reference [15] about the existence of light bullets do not apply in the present case given the lack of translational invariance. Furthermore, It is not obvious that the additional dispersion – introduced by the properties of the Bragg medium – does not lead to a breakdown or collapse of light bullets. The importance of practical applications in

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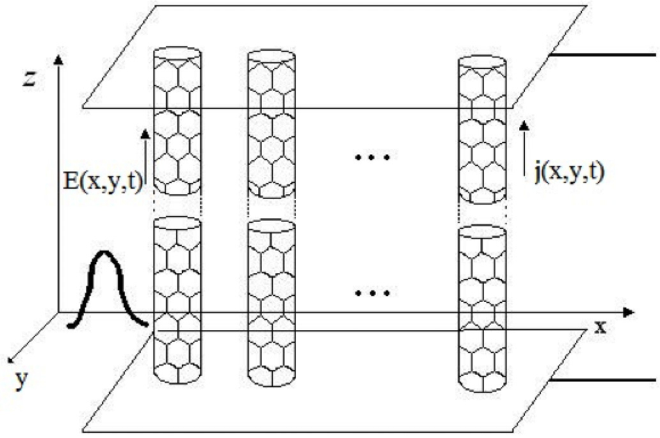

Fig. 1. Geometry of the problem with carbon nanotubes aligned along the z-direction and contributing to generating a Bragg grating along the x-direction.

modern optoelectronics as well as the above considerations have stimulated the present study.

2 Governing equations

The study of the electronic structure of CNTs is usually performed under the strong-coupling approximation and in the framework of the analysis of the dynamics of π-electrons. The dispersion relation for a zigzag-type CNT $(m, 0)$ reads as [10]

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

where $\Delta = 2.7$ 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 precise geometry of the problem considered here is presented in Figure 1. When constructing a model for the propagation of ultrashort optical pulses in a Bragg environment – taking into account the presence of the system of nanotubes – we will describe the electromagnetic field pulse based on Maxwell's equations, using Coulomb's gauge $\mathbf{E} = -\partial\mathbf{A}/c\partial t$ [19]. The vector-potential is thereby expected to take the reduced form $\mathbf{A} = (0, 0, A_z(x, y, t))$. Consequently, the governing propagation equation can be cast as:

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

where $n(x)$ represents the spatial variations of the refractive index, i.e., the Bragg grating; j is the vector 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. Also, the electric field eventually induced by the substrate itself is not considered in this proposed formalism. One additional simplifying assumption has been considered in our model construction, and it consists in discarding possible intergap jumps. This latter simplifying assumption results in restricting the possible frequencies of laser pulses to the near-infrared region. Moreover, we note that 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.

Since a typical relaxation time for electrons in CNTs can be estimated at 3×10^{-13} s, 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 collisionless Boltzmann equation,

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

where $f = f(p_z, s, t)$ is the electron distribution function, which implicitly depends on the spatial coordinates (x, y) through the vector potential $\mathbf{A}(x, y, t)$; q is the electron charge, and c is the speed of light in vacuum. At the initial instant – right before creating the first ultrashort pulse – f is classically given by the equilibrium Fermi-Dirac distribution

$$f_0 = \{1 + \exp\left(E(\mathbf{p})/k_BT\right)\}^{-1},$$

where T is the temperature, and k_B is the Boltzmann constant. The current density $\mathbf{j} = (0, 0, j_z)$ is given by [23]

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

where we have introduced the group velocity $v_z = \partial E(\mathbf{p})/\partial p_z$. Solving equation (3) by means of the method of characteristics allows us to obtain

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

The integration in equation (5) is performed over the first Brillouin zone with $q_0 = 2\pi\hbar/3b$. The group velocity – through which some of the effects of the inhomogeneous dispersion law are imposed to create a Bragg grating – can conveniently be expanded as a Fourier series,

$$v_z(s, x) = \sum_m a_{ms}\sin(mx),$$

where

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

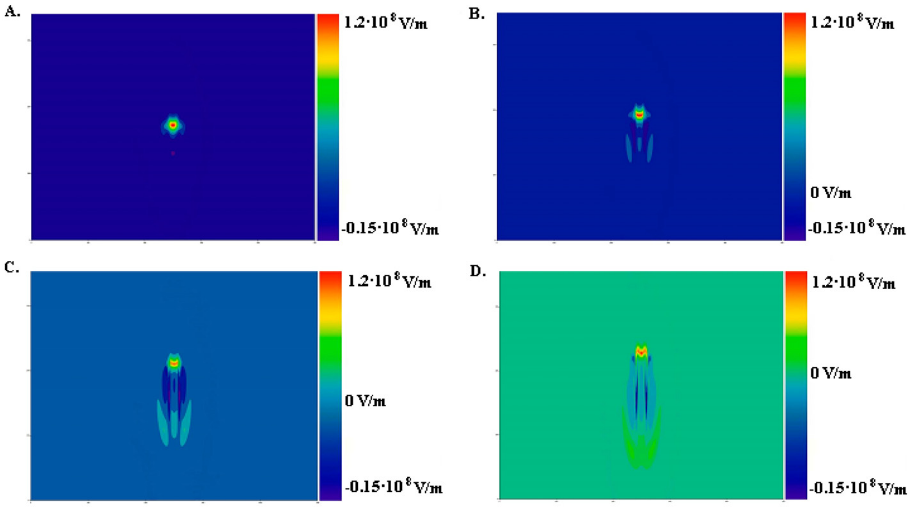

Fig. 2. Propagation of a light bullet in a Bragg medium generated by regularly distributed carbon nanotubes at four different instants in time: (A) $t = T_0$, (B) $t = 2T_0$ (C) $t = 3T_0$ (D) $t = 4T_0$, where $T_0 = 2.5 \times 10^{-12}$ s is the initial period of the light bullet. Values of the field intensity are mapped on a color scale, where the maximum values correspond to red and the minimum ones to purple.

The propagation equation for the vector potential can be recast as

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

where

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

When computing equation (6), as c_m decreases with increasing m, 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 equation (6), we have implemented an explicit finite-difference scheme for hyperbolic equations [24]. 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:

$$A_z(x,y,t=0) = A_0 \exp\left\{-\frac{x^2}{\gamma^2}\right\} \exp\left\{-\beta\left(y-y_0\right)^2\right\}, \tag{7}$$

$$\left.\frac{dA_z}{dt}\right|_{t=0} = \frac{2vx}{\gamma} A_0 \exp\left\{-\frac{x^2}{\gamma^2}\right\} \exp\left\{-\beta\left(y-y_0\right)^2\right\}, \tag{8}$$

where y_0 stands for the center of the bullet, and β is the parameter determining the width of the pulse. The refractive index of the medium has been modeled as $n(x) = n_0(1+\alpha(2\pi x/\chi))$. Here, α is the modulation depth, and χ is the period of the Bragg grating, where we have taken $\alpha = 0.05$ and $\chi = 3 \times 10^{-5}$ m. Note, that we have no grating in the lateral direction.

The simulated shape of the light bullet is shown in Figure 2 at four consecutive instants in time – $t_i = iT_0$ ($i = 1,\dots,4$) – after imposing a pulse corresponding to the initial conditions (7) and (8) at $t = 0$ with period $T_0 = 2.5 \times 10^{-12}$ s. From the evolution of the two-dimensional shape of the propagating light bullet revealed in Figure 2, we can conclude that the spatial modulation of the refractive index in the medium leads to a slowdown of the propagation of light bullets as predicted by the theory. Spatial dispersion also induces significant changes to the shape of the light bullet itself. As can be seen from our computed solution (Fig. 3), the two-dimensional light bullet in our Bragg medium with immersed CNTs remains localized. However, the spatial structure of the pulse evolves over time due to lateral dispersion. The combined effect of the spreading of the pulse associated with dispersion and nonlinearity leads to the formation of a multipeak transverse structure, which nevertheless remains spatially localized.

We have to emphasize that the primary purpose of our study is to show that a steady pulse propagation is still achievable over distances significantly exceeding the pulse size, with a certain level of shape retention. The specific design of the pulse shape minimizing diffractive effects along the transverse direction is beyond the scope of the present work. However, we speculate that super-Gauss pulses should be more stable. These last two issues could be the goals of a separate follow-up study.

Let us summarize the results and conclusions:

(i) Our calculations show that there is a possibility for the propagation of stable two-dimensional light bullets, not only through an array of CNTs [15,20,21,25],

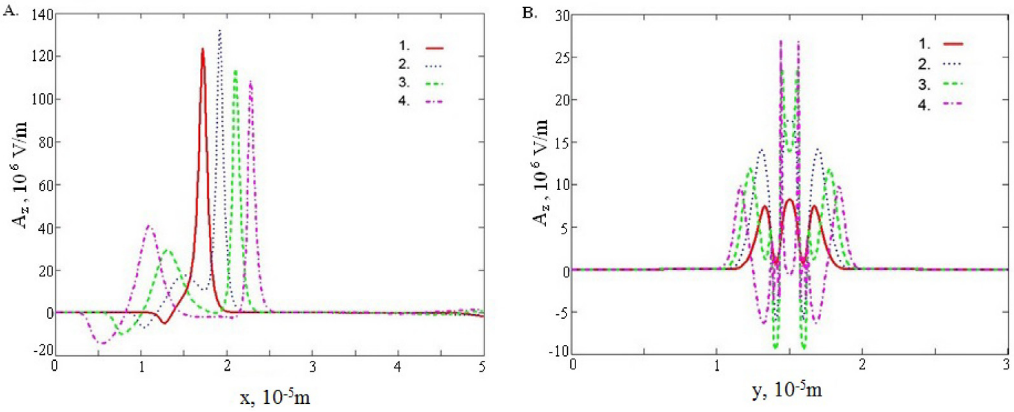

Fig. 3. (A) Spatial variations of the (vector potential) electric field at four consecutive instants in time. In the presence of the Bragg grating, results are given for (1A) $t = T_0$, (2A) $t = 2T_0$, (3A) $T = 3T_0$, (4A) $t = 4T_0$. The dependence of the electric field on the transverse coordinate, y, is presented on (B).

but also through a similar array immersed into a Bragg medium with a spatially and periodically-varying refractive index.

(ii) From a practical viewpoint, our results are important as they demonstrate the possibility to control the propagation speed of light bullets by specifically tuning the parameters defining the Bragg environment.

(iii) Finally, the propagation of light bullets in this Bragg medium with immersed CNTs presents some significant differences from the canonical case of a medium with constant refractive index. Perhaps the most important difference is that light bullets in our Bragg environment bear a more complex transverse structure (Fig. 3). The latter, in our opinion, is due to the excitation of internal vibrational modes of the light bullets because of interactions with the inhomogeneity of the refractive index of the medium.

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