Three-dimensional ultrashort optical Airy beams in an inhomogeneous medium with carbon nanotubes

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ABSTRACT

In this Letter, we consider the problem of the dynamics of propagation of three-dimensional optical pulses (a.k.a. light bullets) with an Airy profile through a heterogeneous environment of carbon nanotubes. We show numerically that such beams exhibit sustained and stable propagation. Moreover, we demonstrate that by varying the density modulation period of the carbon nanotubes one can indirectly control the pulse velocity, which is a particularly valuable feature for the design and manufacturing of novel pulse delay devices.

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1. Introduction

Localized electromagnetic wave packet tends to spread in both space and time under the combined effects of dispersion and diffraction, which are always present in any medium. Over the past two decades, significant research activity has been dedicated to devising new ways to overcome these universal broadening effects in order to generate sustained localized wave packets [1]. Such localized wave packets that are localized in space and that can travel through a medium 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 [2]. However, recent advances in the development of new media with atypical electronic properties have opened new avenues in the generation of sustained propagation of light bullets. In turn, this has generated particular interest in relation with the peculiar nature and dynamics of propagation of these ultrashort optical pulses [3]. Light bullets have also gained significant attention in the field of nonlinear optics owing to potential game-changing applications in modern optoelectronics.

In 2007, Airy optical beams have been achieved by the use of a spatial light modulator [4]. The latter propagates in free space retaining its form at a certain interval, and the trajectory of the main peak is bent recalling the rainbow. It is known that Airy beams have infinite energy (i.e. they are physically unrealizable, but in practice they are approximately generated to some extent) and retain their intensity during the propagation. Thus, Airy beams propagate with an apparent lack of diffractive spreading effects. Moreover, there is increased resistance to amplitude and phase distortions. Other improvements have also been obtained with Airy–Bessel wave packets producing linear light bullets [5]. These unique properties of such optical beams had been captured by earlier pioneering studies based on theoretical analysis [6].

Carbon nanotubes (CNTs) have been used to generate media with unique features as a result of their nonlinear optical properties. CNTs have generated tremendous interest in the research community owing to the simplicity of their structure and their unique properties, which in turn contributed significantly to both the development in optical pulses propagation studies, as well as the development of optical devices based on them. Probably one of the most important feature of CNTs is the ability to use them as a medium for the formation of light bullets [7–11]. Usually the propagation of optical pulses are considered in a uniform CNT environment that does not allow to control the pulse velocity. However, if the propagation velocity of light bullets is determined by the refractive index of the medium and can vary within a wide range, one can perform a further modulation in the refractive index. In turn, this favors the formation of media with a modulated refractive index, thereby enabling the control of the propagation velocity of light bullets as well as the delay time.

As a consequence, various models of propagation of extremely short pulses in a heterogeneous environment have been proposed.
especially given that such an environment makes it possible to control not only the propagation velocity, but also, e.g., the transverse structure of the pulse [12–14]. The most straightforward way to control the input optical field —with CNTs and a spatially modulated refractive index—is to get a nonuniform distribution of CNTs. This leads to a change in the propagation velocity of the optical pulse, and therefore one will be able to control the pulse delay time in such an environment.

Given these recent independent developments in terms of: (i) Airy wave packets as light bullets, and (ii) novel CNT-based inhomogeneous media, it appears timely to investigate the details of the propagation of 3D ultrashort Airy beams in such inhomogeneous media based on CNTs. The present Letter presents the first such study based on a combination of theoretical and numerical analyses.

2. Fundamental equations

Consider the propagation of extremely short optical pulses in an environment of carbon nanotubes, where the electric field is directed along the axis of the nanotubes. The Hamiltonian of the electron subsystem reads

\[ \mathcal{H} = \gamma \sum_{j, \sigma} a_{j \sigma}^\dagger a_{j \sigma} + \text{c.c.}, \]  

where \( a_{j \sigma}^\dagger \) and \( a_{j \sigma} \) are the creation and annihilation operators respectively, for electron with spin \( \sigma \) located at the \( j \)th node, \( \gamma \) is the hopping integral determined by the overlap of the electron wave functions on the neighboring nodes. The abbreviation ‘c.c.’ in Eq. (1) stands for the complex conjugate term. Using the Fourier transform

\[ a_{n \sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_j a_{j \sigma}^\dagger \exp(ijn), \]
\[ a_{n \sigma} = \frac{1}{\sqrt{N}} \sum_j a_{j \sigma} \exp(-ijn), \]

one can easily diagonalize the Hamiltonian by applying a Bogoliubov transformation, thereby yielding the electron spectrum \( \epsilon_\sigma(p) \), which describes the properties of the electronic subsystem in the absence of Coulomb repulsion. For carbon nanotubes of the zigzag type, namely \((m,0)\), the dispersion relation for the energy of conduction electrons reads [15–17]:

\[ \epsilon_\sigma(p) = \pm \sqrt{\left( 1 + 4 \cos^2 \left( \frac{\pi}{m} \right) \right) + 4 \cos^2 \left( \frac{\pi}{m} \right) \left( \frac{s}{m} \right)} \left( \frac{s}{m} \right)^{1/2}. \]

Here, \( s = 1, 2, ..., m \), \( \gamma \approx 2.7 \text{ eV} \), \( a = 3b/2c, b = 0.142 \text{ nm} \) is the distance between adjacent carbon atoms.

Maxwell’s equations in a cylindrical coordinates system can be written as

\[ \frac{\partial^2 \mathbf{E}}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \mathbf{E}}{\partial r} \right) - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \mathbf{E}}{\partial \theta} \right) \left( \frac{4}{c^2} \right) = 0, \]  

where \( \mathbf{E} \) is the electric field of the light wave, \( j \) is the electron current density, \( t \) is the time, and \( c \) is the light velocity in the medium. Let us modify Eq. (4) given our particular choice of the Coulomb gauge, \( \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \). Integrating Eq. (4) over time once, we obtain its generalization for a nonlinear medium as follows

\[ \frac{\partial^2 \mathbf{A}}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \mathbf{A}}{\partial r} \right) - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \mathbf{A}}{\partial \theta} \right) \left( \frac{4}{c^2} \right) = 0. \]

The vector potential \( \mathbf{A} \) and the current density \( j \) are assumed to have the following form \( \mathbf{A} = \{0,0,A(z,r,t)\} \) and \( j = \{0,0,j(z,r,t)\} \), respectively. By solving Eq. (5) for the vector potential \( \mathbf{A} \), one can deduce the current density

\[ j = en(z,r) \sum_{k \sigma} v_\sigma \left( p - \frac{\epsilon}{c} \right) \langle A_{k \sigma}^\dagger A_{k \sigma} \rangle, \]

where \( v_\sigma(p) = \partial \epsilon_\sigma(p)/\partial p \) is the electron group velocity, \( n(z,r) \) is the electron density of CNTs system with possible variations along the radial coordinate \( r \) and the axial coordinate \( z \). Angle brackets denote an average with the nonequilibrium density matrix \( \rho(t) \): 

\[ \langle \theta \rangle = \text{Tr}[\Theta(0)\rho(t)], \]

where \( \Theta \) is the arbitrary dynamic quantity, and \( \text{Tr} \) denotes the trace of a matrix. With account for the conservation law, \( \left\{ \begin{array}{l} \langle A_{k \sigma}^\dagger A_{k \sigma} \rangle, \mathcal{H} \rangle = 0, \text{ the equation of motion for the density matrix} \end{array} \right. \)

\[ \frac{\partial}{\partial t} \langle A_{k \sigma}^\dagger A_{k \sigma} \rangle = \frac{\partial}{\partial t} \langle A_{k \sigma}^\dagger A_{k \sigma} \rangle = 0, \]

where

\[ A_{k \sigma} = \int_{-\pi/a}^{\pi/a} v_\sigma(p) \sin(kp) dp \]

are the coefficients of expansion which decrease with increasing \( k \).

Given that the distribution function \( \rho_0 \) is an even function of the quasi-momentum \( p \), the averaging of \( \sin(kp) \) vanishes, so that

\[ v_\sigma(p) = \frac{\epsilon}{c} \langle A \rangle = \sum_k A_{k \sigma} \cos(kp) \sin \left( \frac{ke}{c} A(t) \right) \]

Substituting Eq. (8) into Eq. (6) and performing the summation over \( s \) and \( p \), we come to

\[ j = -en(z,r) \sum_k B_k \sin \left( \frac{ke}{c} A(t) \right), \]

\[ B_k = \sum_{s=1}^{m} \frac{\pi/a}{1 + \exp(-\beta \epsilon_\sigma(p))} \]

where \( n_0 \) is the equilibrium electron concentration, \( \beta = 1/k_BT \). Note that the current density given by Eq. (9) explicitly contains the nonuniform electron density \( n(z,r) \). Further, in the numerical calculations, this distribution will be given the simple periodic form

\[ n(z,r) = 1 + \alpha \cos \left( \frac{2\pi z}{\chi} \right), \]

where \( \alpha \) is the nonlinearity modulation depth, \( \chi \) stands for the modulation period. Note that in this paper we only consider modulations along the \( z \)-axis.

It is worth noting that due to the field inhomogeneity along certain directions (e.g., the field is directed and nonuniform along the \( z \)-axis), the current is also not uniform. The heterogeneity of the current causes an accumulation of charges in some areas that can be assessed from the charge conservation law:
\[ \frac{d\rho}{dt} + \frac{dj}{dz} = 0. \]  
\[ \rho \propto \tau \frac{j}{I_z}. \]  

Here \( \rho \) is the charge density, \( j \) is the current density along the z-axis, \( \tau \) is the pulse duration, and \( I_z \) is the characteristic length for the electric field change along the z-axis. Equation (11) allows us to conclude that the duration of a short pulse has a significant impact on the accumulated charge. Our estimates show that the accumulated charge is about 1–2% of the charge, which contributes to the current. The latter allows one to neglect the charge accumulation effect for femtosecond pulses. This approximation has been validated by other numerical experiments for the case of CNTs and a pulse duration of tens of femtoseconds [9,12,15–17].

3. Results and discussion

Equation (5) is solved numerically with the assumption of the inter-band current to be zero. In other words, we assume that the spectrum of the light bullet lies above the visible spectrum and the maximum oscillation frequency of the light bullet spectrum is in the near infrared region. Steps in time and coordinates are determined from the stability conditions. They where decreased as long as the solution is not changed in the eighth decimal place. The initial condition for the vector potential of the electric field was chosen as follows:

\[ A(z, r, t = 0) = Q R \left\{ \frac{z - z_0}{\gamma_z} + \frac{z - z_0}{\gamma_z} \right\} \frac{\hat{r}}{r} \left\{ 0 \right\} \exp \left( - \frac{r}{\gamma_r} \right). \]

\[ dA(z, r, t = 0) \]

\[ \frac{dA(z, r, t)}{dt} = Q \frac{d}{dt} R \left\{ \frac{z - z_0 - ut'}{\gamma_z} + \frac{z - z_0 - ut'}{\gamma_z} \right\} \left\{ 0 \right\} \exp \left( - \frac{r}{\gamma_r} \right) \]

\[ \times \left\{ \frac{r}{r} \right\} \frac{\hat{r}}{r} \left\{ \frac{r}{r} \right\} \exp \left( - \frac{r}{\gamma_r} \right). \]

\[ R(x) = \int_{\chi} A_0(y)dy. \]

Here \( Q \) is the pulse amplitude, \( \gamma_z \) and \( \gamma_r \) are the widths of the pulse in the z- and r-direction respectively; \( u \) is the initial pulse velocity; \( \kappa \) is a parameter—we denote it as the Airy parameter of the pulse in what follows; \( \gamma \) is a cutoff parameter, which is introduced to make the pulse physically implementable, so that it carries a finite amount of energy; \( J_0 \) is the Bessel function of the first kind.

Results for the pulse propagation over time are shown in Fig. 1. As can be seen from the figure, the Airy pulse propagates steadily. Most of the energy continues to be concentrated in the central part of the pulse, although there is a slight broadening due to diffraction. Clearly, the light bullets show stability while propagating through this medium. Note that unlike the case of a linear medium, in the present case—due to the nonlinearity of the medium—the pulse shape is not retained anymore.

The dependence of the pulse shape on the parameter \( \kappa \) of the Airy function is shown in Fig. 2. From the above consideration, it is clear that the parameter \( \kappa \) of Airy function affects the structure of the pulse, although the pulse itself is still localized regardless of the value of \( \kappa \).

The dependence on the density modulation period of nanotubes is shown in Fig. 3. As expected, the increase in the modulation period leads to the propagation of the pulse with a larger velocity, while a decrease in the modulation period reduces the speed of the pulse, respectively. This is in general agreement with the concept of pulse formation and behavior in a periodically modulated medium. One can say that by changing the period of modulation of the density of carbon nanotubes, one gains indirect control over the pulse velocity. This latter feature is of tremendous importance given its potential valuable applications in manufacturing pulse delay devices.

4. Conclusions

Key results of this work may be summarized as follows:

i) We studied the propagation of ultrashort Airy optical pulses in a heterogeneous environment formed by an array of carbon nanotubes with a periodically modulated density. Our analysis demonstrates the possibility for the stable propagation of light bullets. As expected, the heterogeneity of the environment to a large extent affects the pulse shape, namely smoothing it.

ii) It was established that the Airy function parameter has a non-negligible effect on the pulse structure. However, the pulse does remain localized, regardless of the value of the Airy parameter.

iii) It is proved that changes in the modulation parameter—through the lattice constant in the present study—allow one to control the pulse propagation. An increase in the modulation period results in an increase of the pulse propagation velocity.
**Fig. 2.** Electric field distribution during the propagation of ultra-short Airy pulse through the array of carbon nanotubes (lattice constant is $\chi = 0.05 \mu m$; $r$ and $z$ are in $\mu m$) at $T = 6$ ps for different values of the parameter $\kappa$ ($k_0 = 0.25$): (A) $\kappa = 0.05k_0$; (B) $\kappa = 0.07k_0$; (C) $\kappa = 0.08k_0$; (D) $\kappa = 0.1k_0$; (E) $\kappa = 0.3k_0$; (F) $\kappa = 0.5k_0$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

**Fig. 3.** Electric field distribution during the propagation of ultra-short Airy pulse through the array of carbon nanotubes (lattice constant is $\chi = 0.05 \mu m$; $\kappa = 0.01$; $r$ and $z$ are in $\mu m$) at $T = 6$ ps for different values of the parameter $\kappa$ ($k_0 = 0.25$): (A) $\kappa = 0.05k_0$; (B) $\kappa = 0.07k_0$; (C) $\kappa = 0.08k_0$; (D) $\kappa = 0.1k_0$; (E) $\kappa = 0.3k_0$; (F) $\kappa = 0.5k_0$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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