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Three-dimensional extremely-short optical pulses in carbon nanotube arrays in the presence of an external magnetic field

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In this paper, we study the behavior of three-dimensional extremely-short optical pulses propagating in a system made of carbon nanotubes in the presence of an external magnetic field applied perpendicular both to the nanotube axis and to the direction of propagation of the pulse. The evolution of the electromagnetic field is classically derived on the basis of the Maxwell's equations. The electronic system of carbon nanotubes is considered in the low-temperature approximation. Our analysis reveals the novel and unique ability of controlling the shape of propagating short optical pulses by tuning the intensity of the applied magnetic field. This effect paves the way for the possible development of innovative applications in optoelectronics.

Keywords: CNTs; ultra-short pulses; magnetic fields.

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1. Introduction

Since the discovery of carbon nanotubes (CNTs),[1] this material has attracted the attention of many researchers studying the related structures both theoretically and experimentally. Due to the stable structure and unique electrical properties, CNTs have been the object of attention in the field of nonlinear optics, as well as among the developers of various electronic nanodevices.[2] It should be noted that the scope

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of nanoelectronic devices based on CNTs can be quite broad, for example, nanoengineering, medical diagnostic and medical practice, biomedical laser technology, just to name a few.

Despite the significant number of studies on the dynamics of both one-dimensional and two-dimensional electromagnetic waves in systems of carbon nanostructures (see, for example, Refs. 3–5 and references therein), to this day there remain many unexplored issues related to the influence of external electrical and magnetic fields on the propagation of three-dimensional extremely-short pulses in the system of CNTs.

It should be noted that the effect from static magnetic field may be even more significant than the effect of static electric field due to the fact that a constant magnetic field, as shown in Ref. 6, can greatly change the single electron spectrum. In this paper, an attempt is made to consider the effect of such a constant magnetic field on the dynamics of three-dimensional extremely-short optical pulses propagating through an array of CNTs. Specifically, it is interesting solving the problem of propagation of ultrashort pulses in the case when the constant magnetic field is perpendicular to the axis of the carbon nanotubes.

All of the above circumstances provide the impetus for this study. Specifically, we demonstrate that by varying the external constant magnetic field, one can tune the dispersion law of free electrons in the CNTs, and in turn, indirectly control the propagation of femtosecond optical pulses in the environment. The latter is of paramount importance in both technology and medical applications.[7]

2. Formulation of the Problem and Governing Equations

A study of the electronic structure of carbon nanotubes was carried out in the framework of the analysis of the dynamics of π-electrons in the strong-coupling approximation. For the CNTs of zigzag type $(m, 0)$, the electron dispersion law in the presence of a magnetic field H parallel to the nanotube axis is given by[6]

$$\epsilon_s(k_x, k_z, H) = \pm\gamma \left\{ 1 + 4\cos\left(\frac{\sqrt{3}ak_x}{2}\right)\cos\left(\frac{3ak_z}{2}\right) + 4\cos^2\left(\frac{\sqrt{3}ak_x}{2}\right)\right\}^{1/2}, \quad (1)$$

where $a = 1.4$ Å, $\gamma \approx 2.7$ eV, k_z is the wave vector along the nanotube axis, while k_x is the wave vector along the x-direction, which is dependent on the intensity H of the magnetic field according to

$$k_x(H) = \frac{2\pi}{\sqrt{3}am}\left(s + \frac{\Phi(H)}{\Phi_0}\right),$$

where $\Phi(H)$ is the magnetic flux through the cross-section of the tube, $\Phi_0 = \hbar c/e$ and $s = 1, 2, \ldots, m$.

In this paper, we consider the propagation of ultrashort electromagnetic pulses in a system of CNTs in the geometry depicted in Fig. 1, where the external magnetic field is applied perpendicular to the axis of nanotubes. In this case, it is natural to

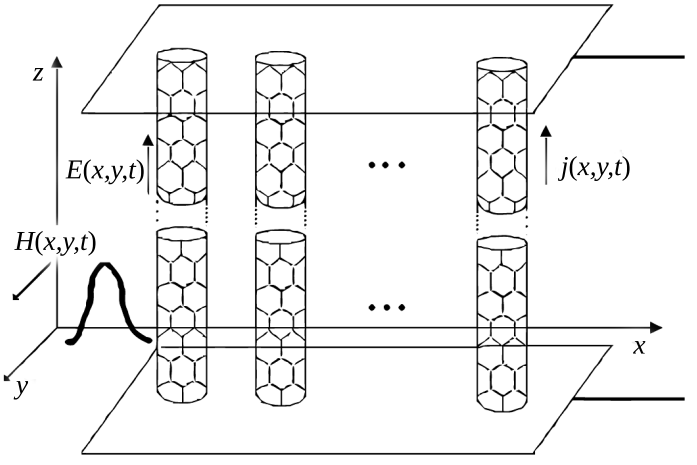


Fig. 1. Schematic diagram of the geometry of the studied problem with the axis of CNTs oriented parallel to the z-direction.

use the classical Peierls substitution.[8] In this case, the vector potential reads

$$\mathbf{A}_0 = \left(-\frac{Hy}{2}, \frac{Hx}{2}, 0\right),$$

and is fully determined by the constant magnetic field H. The vector potential must be included into the phase factor of the Hamiltonian for electrons hopping between neighboring nodes of the hexagonal nanotube structure. Hence, the Hamiltonian reads

$$\mathcal{H} = \frac{1}{2}\sum_{n,m} \gamma_{nm} a_n^\dagger a_m + \text{c.c.}, \tag{2}$$

where

$$\gamma_{nm} = \gamma \exp\left(i\frac{\Phi_{\text{eff}}}{\Phi_0}\right), \quad \Phi_{\text{eff}} = \int_{\mathbf{r}_n}^{\mathbf{r}_m} \mathbf{A}_0 d\mathbf{r}\,.$$

Here $\mathbf{r}_n$ and $\mathbf{r}_m$ stand for the point vectors of the corresponding neighboring atoms of CNT, and the integration is carried out along the bond between the atoms; $a_n^\dagger$ and a_m are the electron creation and annihilation operators, respectively.

Unfortunately, the Hamiltonian (2) cannot be diagonalized analytically (because of dependence on the spatial indexes), bit still can be diagonalized numerically, thereby obtaining the dispersion law. The obtained dispersion law $\Delta(k_z, s)$ depends on two variables, k_z and s. The quantity k_z takes values in the first Brillouin zone, and it is associated with the electron momentum directed along the nanotube axis. The index s is due to the quantization of movement along the tube circumference and takes values as in Eq. (1). Note that the specific form $\Delta(k_z, s)$ is not important for our further analysis, but only the coefficients of its expansion in a Fourier series with respect to k_z are.

Using the standard Coulomb gauge (see Ref. 9) $\mathbf{E} = -\frac{1}{c}\partial\mathbf{A}/\partial t$, we can write the Maxwell's equations as follows[10]:

$$\frac{\varepsilon}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} - \frac{\partial^2\mathbf{A}}{\partial x^2} - \frac{\partial^2\mathbf{A}}{\partial y^2} - \frac{\partial^2\mathbf{A}}{\partial z^2} - \frac{4\pi}{c}\mathbf{j} = 0\,, \tag{3}$$

where the vector potential is assumed to have the form $\mathbf{A} = \{0, 0, A(x,t)\}$.

Here, we aim to derive an expression for the conduction-current density j, applying an approach similar to the one used in Refs. 12 and 13 for semiconductor superlattices. Expanding the dispersion relation in a Fourier series, one can write the expression for the projection of the current density on the x-axis within the collisionless approximation:

$$j = -en\frac{a}{\hbar}\gamma\sum_{s=1}^{m}\sum_{r=1}^{\infty}G_{r,s}\sin\left\{re\frac{aA}{c\hbar}\right\}, \tag{4}$$

where e is the electron charge and n is the concentration of the conduction electrons in the array of carbon nanotubes. Note that the coefficients $G_{r,s}$ are given by

$$G_{r,s} = -r\frac{\delta_{r,s}}{\gamma}\frac{\int_{-\pi}^{\pi}\cos(r\xi)\exp\{-\sum_{r=1}^{\infty}\theta_{r,s}\cos(r\xi)\}d\xi}{\int_{-\pi}^{\pi}\exp\{-\sum_{r=1}^{\infty}\theta_{r,s}\cos(r\xi)\}d\xi}\,, \tag{5}$$

where $\theta_{r,s} = \delta_{r,s}(k_BT)^{-1}$, and

$$\delta_{r,s} = \frac{a}{\pi\hbar}\int_{-\pi\hbar/a}^{\pi\hbar/a}\Delta(k_z,s)\cos\left(r\frac{a}{\hbar}k_z\right)dk_z\,. \tag{6}$$

It is worth noting that the coefficients $G_{r,s}$ decrease rapidly with increasing r, approximately like $(1/2)^r$.

The current density j, given by Eq. (4), explicitly depends on the vector potential $\mathbf{A}$. Substituting Eq. (4) into Eqs. (2) and (3), we obtain an equation describing the evolution of the electromagnetic field pulse in the CNTs system:

$$\frac{\partial^2\Psi}{\partial\tau^2} - \left(\frac{\partial^2\Psi}{\partial\xi^2} + \frac{\partial^2\Psi}{\partial\nu^2} + \frac{\partial^2\Psi}{\partial\zeta^2}\right) + \eta\sum_{s=1}^{m}\sum_{r=1}^{\infty}G_{r,s}\sin(r\Psi) = 0\,. \tag{7}$$

Here $\Psi = Aed_x/c\hbar$ is the dimensionless projection of the vector potential on the x-axis, $\tau = \omega_0 t/\sqrt{\varepsilon}$ is the dimensionless time, $\xi = \omega_0 x/\sqrt{\varepsilon}$, $\nu = \omega_0 y/\sqrt{\varepsilon}$ and $\zeta = \omega_0 z/\sqrt{\varepsilon}$ are the dimensionless spatial coordinates.

It is important to note the following point. As a consequence of the field inhomogeneity along some axis (e.g. the field is directed and is non-uniform along the z-axis), the current is also non-uniform. The heterogeneity of the current causes the accumulation of charges in some areas that can be estimated from the charge conservation law

$$\frac{d\rho}{dt} + \frac{dj}{dz} = 0\,, \tag{8}$$

$$\rho \propto \tau\frac{j}{l_z}\,. \tag{9}$$

Here ρ is the charge density, j is the current density along the z-axis, τ is the pulse duration and l_z is the characteristic length on which the electric field is measured. Equation (9) allows us to conclude that a significant impact on the accumulated charge comes from a maximum duration of a short pulse. The estimates show that the accumulated charge is about 1–2% of the total charge, which contributes to the current. The latter allows us to neglect the charge accumulation effect for femtosecond pulses. This is confirmed by numerical experiments for the case of carbon nanotubes and a pulse duration of tens of femtoseconds.[11,14,15]

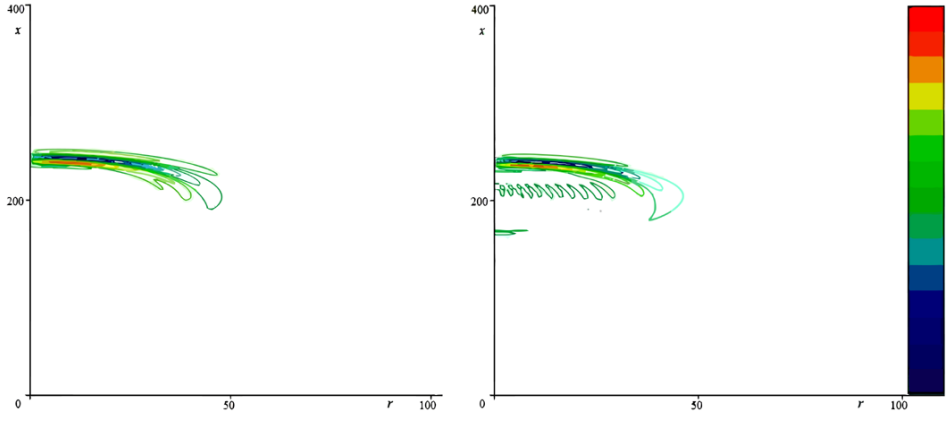
3. Results of the Numerical Analysis

Equation (7) has been solved numerically using the explicit finite difference cross-type schemes[16] with temporal evolution. Spatial and temporal steps were determined from the well-known and standard stability conditions.[16] Both spatial and temporal convergences were achieved by successively halving the space and time steps until the computed solution remains unchanged up to the eighth decimal place. The constant magnetic field was initially assumed to be zero. The following initial conditions were selected:

$$\Psi = Q \exp\left\{-\left(\frac{x - vt}{\gamma\Delta}\right)^2\right\} \exp(-\beta^2 r^2)\,,$$
$$\gamma = (1 - v^2)^{1/2}, \quad r^2 = y^2 + z^2\,, \tag{10}$$

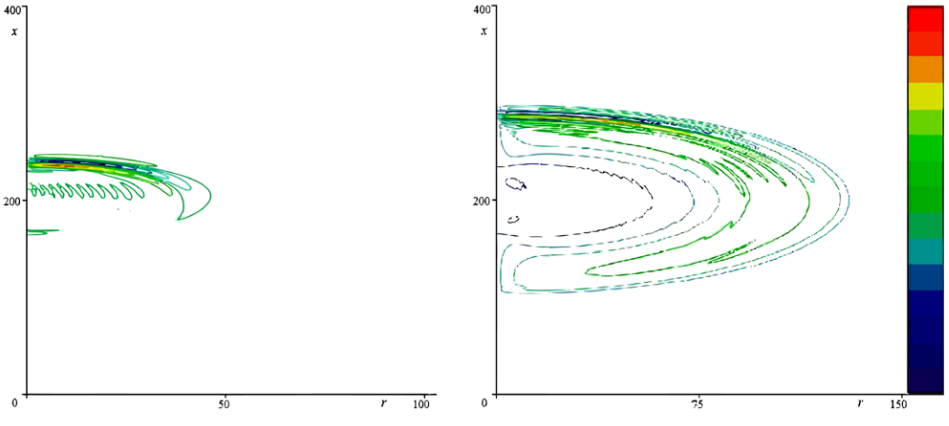
where Q is the initial pulse amplitude, Δ is the half-width of the initial pulse, r defines the transverse structure of the pulse in space, γ and β are the parameters determining the pulse widths in the x- and r-directions, respectively, and v is the initial pulse velocity. The speed of light is taken as being unity in numerical simulations. It should be noted that in the considered electronic system of CNTs, the typical characteristic relaxation time is of the order of 10^{-11} s, while the extremely-short pulse in our problem has a duration of about 10^{-15} s. Thus, this approach may be applicable to the time of the order of 10^{-12} s, which corresponds to a short pulse traveling a maximum distance of the order of 10^{-4} m, that may well be achieved in the experiment.

The evolutions of the three-dimensional very short pulse in the carbon nanotubes system in the absence and presence of an external magnetic field are shown in Fig. 2. As can be seen from the figures, three-dimensional extremely-short pulses propagating in the medium made of CNTs under the influence of a magnetic field experience a change in their spatial structure due to changes in the dispersion relation. Specifically, the magnetic field applied perpendicular to the axis of CNT affects the dispersion law, which in turn affects the actual propagation of the three-dimensional extremely-short pulses, and eventually leads to changes in its shape.



(a) (b)

Fig. 2. (Color online) Coordinate profiles of the electric field intensity of the three-dimensional extremely-short optical pulse in the system of carbon nanotubes under the influence of an external magnetic field at the time $T = 6$ ps. The electric field intensity is mapped onto a color scale, the maximum values of the field intensity correspond to red and the minimum ones to purple. (a) Profile in the absence of any magnetic field and (b) that under an applied magnetic field such that $\Phi_{\text{eff}}/\Phi_0 = 1.1$. Note that $v/c = 0.98$, and the units on both axes correspond to 3×10^{-8} m.



(a) (b)

Fig. 3. (Color online) Coordinate profiles of the electric field intensity of the three-dimensional extremely-short optical pulse in the system of carbon nanotubes under the influence of an external magnetic field at different instances of time. The electric field intensity is mapped onto a color scale, the maximum values of the field intensity correspond to red and the minimum ones to purple. (a) Profile at $T = 6$ ps and (b) the one at $T = 18$ ps. Here $v/c = 0.98$ and $\Phi_{\text{eff}}/\Phi_0 = 1.1$. The units on both axes correspond to 3×10^{-8} m.

With an increase in the time of propagation of the pulse we observe the evolutions shown in Fig. 3. From these plots, one can notice that increasing the pulse propagation time in the presence of an applied magnetic field, changes significantly the pulse shape. Moreover, the pulse becomes less localized in space and separates into several daughter pulses, which have substantially different amplitudes.

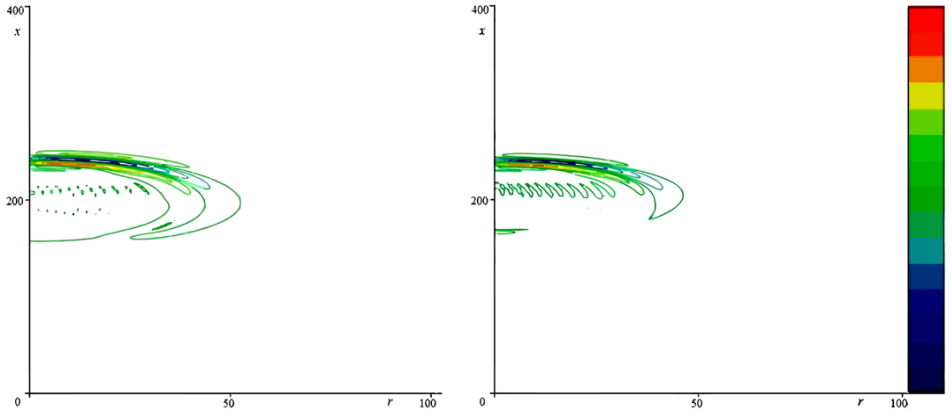


Fig. 4. (Color online) Coordinate profiles of the electric field intensity of the three-dimensional extremely-short optical pulse in the system of carbon nanotubes for different values of the applied magnetic field at $T = 6$ ps. The electric field intensity is mapped onto a color scale, the maximum values of the field intensity correspond to red and the minimum ones to purple. (a) Profile for $\Phi_{\text{eff}}/\Phi_0 = 0.55$ and (b) the one for $\Phi_{\text{eff}}/\Phi_0 = 1.1$. Here $v/c = 0.98$. The units on both axes correspond to 3×10^{-8} m.

Also, it should be noted that the three-dimensional extremely-short pulse changes its configuration not only over time, but also as a result of dispersion effects. Figure 4 reveals the solutions of Eq. (7) depending on two different values of the applied constant magnetic field. As one would expect, variations of the external magnetic field lead to changes in the pulse shape. In particular, an increase in the applied magnetic field increases both the amplitude and the magnitude of the observed localization in the space of the pulse.

4. Conclusions

In conclusion, we note that all the key effects arising from the introduction of an external magnetic field directed perpendicular to the axis of carbon nanotubes, are due to induced changes in the dispersion law of the electrons. This dispersion law is entirely responsible for the observed vast range of dynamics of the propagation of ultrashort three-dimensional pulses. Thus, it can be concluded that the dispersion law of free electrons in the carbon nanotubes, in particular, in the presence of a constant magnetic field, governs the propagation of the optical pulses in the environment. And thus, it can be argued that it is possible to control the shape of three-dimensional extremely-short optical pulse propagating in an environment of carbon nanotubes by a tuning of the applied constant magnetic field.

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