Optical pulses in carbon nanotubes with strong electron-electron interaction due to impurities

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Abstract. In this paper, we investigate electromagnetic pulse propagation in a medium with impurity carbon nanotubes, which are associated with the acoustic subsystem. The electron spectrum for the carbon system is obtained from the model that takes into account Coulomb impurities. Based on the Maxwell's and the wave equations for the vector of the medium displacements, we obtain the effective equations for the vector potential of the electromagnetic field and the component of the displacement vector of the medium. The dependence of the pulse shape on the various system parameters is analyzed.

1. Introduction
In recent years, there has been an increasing interest in impurities, which leads to a change in the properties of materials [1–3]. An interest in such topics may be associated with modern trends in opto-, micro- and microwave electronics, since it becomes necessary to control the energy spectrum of electrons. Obviously, the existence of various kinds of impurities and the nature of their interaction with the system requires the use of various approaches (for example, [4–5]).

At the same time, it is important to take into account the properties of the medium in which the carbon nanotubes (CNTs) are placed, since, different properties (piezoelectric, magnetic, ferroelectric, etc.) can have a significant effect on the electromagnetic wave propagation. Therefore, this work is devoted to the study of ultrashort optical pulses in a medium with impurity carbon nanotubes, and the CNTs are associated with an acoustic subsystem.

In this case, we use the model described in [6]. It takes into account the strong electron-electron interaction caused by the return of electrons from impurities to the electron system of CNTs. Thus, the Fermi velocity is renormalized, which has a logarithmic dependence on the electron energy. Earlier [7] we have already applied this model, but without taking into account the properties of the environment itself.

2. Model
We consider the propagation of the ultrashort electromagnetic pulses in doped carbon nanotubes (it is assumed that electrons pass into the carbon system of CNTs with impurities), taking into account the finite mass of quasiparticles. For definiteness, we direct the electric field of the pulse along the CNT axis (z-axis).

The dispersion law for carbon nanotubes with a strong electron-electron interaction can be found according to the well-known relationship between the charge velocity and the electron energy: $v_z = \frac{\partial \varepsilon(q_x,q_z)}{\partial q_z}$.

According to Ref. [6] we can write:
Here \( q_x, q_z \) are the electron momentum components, \( \Lambda \) is the spectrum gap (0.1 eV).

According to the quantum mechanics rules in the presence of the electric field \( E \), which is directed along the \( z \)-axis and is considered in calibration: \( E = -\frac{\partial A}{c \partial t} \), it is necessary to replace the momentum with a generalized one: \( q \rightarrow q - eA/c \) (\( e \) is the electron charge, \( c \) is the light velocity).

The Maxwell's equations, taking into account the calibration, in the two-dimensional case can be written in the following form [8]:

\[
\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial z^2} - \frac{1}{c^2} \frac{\partial^2 A}{\partial t^2} + \frac{4\pi}{c} j = \beta \frac{\partial P}{\partial t}
\]

The vector potential has the following form \( A = (0,0,A(x,z,t)) \), and the current density \( j \) is \( j = (0, 0, j_z) \).

To take into account the properties of the medium, we supplemented Eq. (2) with the term with medium polarization \( P \), directed along the CNT axis.

Let us write the standard expression for the current density:

\[
j = e \sum_{q_v} v \left( q - \frac{e}{c} A(x,z,t) \right) \langle a_q^* a_q \rangle
\]

where the brackets denote averaging with a nonequilibrium density matrix \( \rho(t) \): \( \langle B \rangle = \text{Sp} \left\{ B(0) \rho(t) \right\} \).

Taking into account \( \left[ a_{q_v}^* a_{q_v}, H \right] = 0 \) from the equations of motion for the density matrix we obtain that:

\( \langle a_{q_v}^* a_{q_v} \rangle = \langle a_{q_v}^* a_{q_v} \rangle_0 \), where \( \langle B \rangle_0 = \text{Sp} \left\{ B(0) \rho(0) \right\} \). Thus, in the expression for the current density, one can use the number of particles that follows from the Fermi-Dirac distribution. Next, we consider the case of low temperatures, when only a small part contributes to the sum in momentum space near the Fermi level. So, we write formula (3) in the form:

\[
j = e \int_{-\Delta}^{\Delta} dq_v \int_{-\Delta}^{\Delta} dq_x v \left( q - \frac{e}{c} A(x,z,t) \right)
\]

The region of integration over momenta in (4) is determined from the equality condition of the number of particles:

\[
\int_{-\Delta}^{\Delta} dq_x dq_v = \int_{-\Delta}^{\Delta} dq_x dq_v \left\langle a_{q_v}^* a_{q_v} \right\rangle
\]

Integration on the right is carried out over the first Brillouin zone.

In this case, the equation for the nonzero component of the vector potential can be written as:

\[
\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial z^2} - \frac{1}{c^2} \frac{\partial^2 A}{\partial t^2} + \frac{4\pi}{c} F(A + \eta) = \beta \frac{\partial P}{\partial t},
\]

\( F(A) \) is determined by integration in (4). The quantity \( \eta \) is related to the nonzero component of the displacement vector of the medium \( u \) as:

\[
\eta = -cd \int_0^{t} \frac{\partial u(z,t')}{\partial z} dt'.
\]
\[ P = d \frac{\partial u}{\partial z} \]  \hfill (7)

\( d \) is the piezomodule.

The equation (5) in this case must be supplemented with the equation for the component of the displacement vector \( u \) [9-10]:

\[ \frac{\partial^2 u}{\partial t^2} + \gamma \frac{\partial u}{\partial t} + \omega_0^2 u = \chi \frac{\partial A}{\partial t} \]  \hfill (8)

here \( \gamma \) is the heavy ion absorption coefficient, \( \omega_0 \) is the heavy ion resonance frequency, and \( \chi \) is the susceptibility coefficient. Let us note several used approximations. First, only one component of the displacement vector is taken into account. Second, we consider the polarization vector collinear to the electric field vector.

3. Numerical simulation results

The investigated equation (5) is solved numerically using a direct difference scheme of the cross type [11]. The initial condition is chosen in Gaussian form and can be written as:

\[ A(x, z, 0) = Q \exp \left( -\frac{(z - z_0)^2}{l_z^2} \right) \exp \left( -\frac{(x - x_0)^2}{l_x^2} \right), \]

\[ \frac{dA(x, z, 0)}{dt} = 2Qv_0 \frac{z - z_0}{l_z^2} \exp \left( -\frac{(z - z_0)^2}{l_z^2} \right) \exp \left( -\frac{(x - x_0)^2}{l_x^2} \right), \]  \hfill (9)

\[ u(x, z, 0) = 0, \quad \frac{du(x, z, 0)}{dt} = 0 \]

where \( Q \) is the pulse amplitude, \( v_0 \) is the initial velocity of the pulse, \( l_x, l_z \) determine the pulse width along the x and z directions, respectively, and \((x_0, z_0)\) is the initial position of the pulse.

Figure 1 demonstrates the evolution of the electromagnetic wave during its propagation over the sample.
Figure 1. The intensity of the electric field of the pulse: a) $t=0$; b) $t=3 \cdot 10^{-14} \, s$; c) $t=6 \cdot 10^{-14} \, s$; d) $t=9 \cdot 10^{-14} \, s$; e) longitudinal sections for the figures (a-d) at $x=0$. $I_{\text{max}}$ is the maximum intensity value at $t=0$. The nondimensional unit along the $x$ and $z$ axes corresponds to $2 \cdot 10^{-5} \, m$.

It can be seen, that the pulse propagation is rather stable and is accompanied by dispersion in the transverse direction. Note that this behavior of the pulse is due to the nature of nonlinearity, since the dependence of the current on the potential is of a saturating nature, which counteracts the destruction of the pulse. Its division into several pulses is also observed along with a decrease in the amplitude of each pulse, which is associated with strong dispersion in the system due to the interaction with the acoustic subsystem.

We investigate the effect of the piezo module $d$ on the process of pulse propagation over the sample (Fig. 2).

Figure 2. The intensity of the electric field of the pulse (at $t=9 \cdot 10^{-14} \, s$):
For curve 2, the piezo module is 2 times greater than for curve 1. For curve 3, the piezo module is 3 times larger than for curve 1. (a) longitudinal sections at $x=0$, (b) cross sections passing through the maximum. $I_{\text{max}}$ is the maximum intensity value at $t=0$.

The nondimensional unit along the $z$ axis corresponds to $2 \cdot 10^{-5} \, m$. 
In accordance with figure 2, the larger the value of d, the stronger the transverse dispersion of the pulse due to the piezoelectric effect. That is, one can control the pulse width by changing the magnitude of the piezo module. This is due to the fact that the electric field of the pulse is associated through the piezoelectric effect with the motion of heavy ions. In turn, heavy ions experience damping of motion during pulse propagation. Therefore, with an increase in the coupling between the pulse field and heavy ions, most of the pulse energy is transferred to the kinetic energy of the motion of heavy ions. Due to dissipation (coefficient \( \gamma \) in equation (8)), energy is converted into heat and heats the sample. And the pulse amplitude also decreases. So, we can conclude that for practical applications it is necessary to use nanotubes in media with the lowest piezomodule value.

Conclusions
The study results in the following conclusions:

- An ultrashort optical pulse in carbon nanotubes with a strong electron-electron interaction is shown to propagate steadily, which is explained by the balance of dispersion and nonlinearity.
- The magnitude of the piezo module is a control parameter for the ultrashort pulse that allows controlling its transverse broadening.
- Carbon nanotubes easily trap impurities that donate their electrons to the tubes and this has a stabilizing effect on the ultrashort pulse propagating in a piezoelectric medium with CNTs. Therefore, such media can be used in the development of waveguides and delay devices.

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