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Dynamics of extremely short pulses in two-level impurity systems in the framework of the glauber approach[1]

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In this work, we study the features of the propagation of extremely short optical pulses in a two-level system using the example of a deuterated ferroelectric containing carbon nanotubes. Based on the Heisenberg equation of motion for the average values of the pseudospin operators, as well as the wave equation for the electric field, a numerical simulation of the dynamics of an electromagnetic pulse is carried out. The evolution of the system for various parameters of the problem is demonstrated.

Keywords: extremely short pulse, two-level system, carbon nanotubes.

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Introduction

The interest of researchers in the effects that arise in a nonlinear medium when interacting with a laser radiation field is due to both recent theoretical and practical achievements [1–3]. These successes are primarily associated with obtaining stable light structures that are localized in a limited region of space [4]. In this case, an important issue is the study of the stability of light pulses [5], including by searching for a suitable medium.

In this work, we propose to use a deuterated ferroelectric medium. It is widely known that ferroelectrics are a convenient means of studying structural phase transitions (PT) by experiencing a PT of the second kind „order−disorder“ [6]. This allows you to control their properties by changing the temperature [7]. Note also that a two-level system is the simplest quantum model that is used in studying the interaction of light with matter. It remains attractive until now in the field of nonlinear optics, in particular, for determining the conditions for the generation of various optical solitons [8].

Note that to ensure a stable state of optical pulses, we introduce carbon nanotubes (CNTs) [9] into the medium, which have shown themselves well in this matter [10,11], starting from their pioneering work jcite12.

Model and basic equations

We assume that the CNT axes are codirectional with the OZ axis, the wave vector is directed along the OY axis. Let's study the dynamic properties of the system under consideration within the framework of Glauber's approach [13]. The kinetic equation for describing the pseudospin dynamics can be written [14] as

$$\langle\dot{S}\rangle = -\frac{\langle S\rangle - 0.5\tanh\left(\beta(J\langle S\rangle + \Delta_{\perp}\langle S\rangle\alpha + \gamma\langle S\rangle_{zz} + \delta E)\right)}{T_{\mathrm{imp}}}, \tag{1}$$

where T_{imp} -is relaxation time, α, γ are constants determined by the magnitude of the exchange interaction, J is energy of the Coulomb interaction, $\langle S\rangle$ is average value of the pseudospin, here the dot denotes the time derivative, $\Delta_{\perp}$ is- the Laplacian in the direction perpendicular to the CNT axis, $\beta = 1/k_B T$, k_B is Boltzmann constant, T is temperature, δ is dipole moment, E is electric field along CNT axis.

Maxwell's equations for the electric field component directed along the nanotube axes can be written in the following form:

$$\frac{1}{c^2}\frac{\partial^2 E}{\partial t^2} - \nabla^2 E = -\mu\langle\ddot{S}\rangle + \frac{4\pi}{c}\frac{\partial j}{\partial t}, \tag{2}$$

where c is the speed of light, μ is a constant related to the polarization of the impurity system.

Taking into account the gauge $\mathbf{E} = -\partial\mathbf{A}/c\partial t$ and the form of the vector potential $\mathbf{A} = (0, 0, A(x, z, t))$, as well as the electric current density $\mathbf{j} = (0, 0, j(x, z, t))$, equation (2) can be rewritten as follows:

$$\frac{1}{c^2}\frac{\partial A}{\partial t^2} - \nabla^2 A = -\mu\cdot\langle S\rangle + \frac{4\pi}{c}j(A). \tag{3}$$

Note that in the three-dimensional case, taking into account $\mathbf{A} = (0, 0, A(x, y, z, t))$ and the transition to a cylindrical coordinate system, equation (3) will be as

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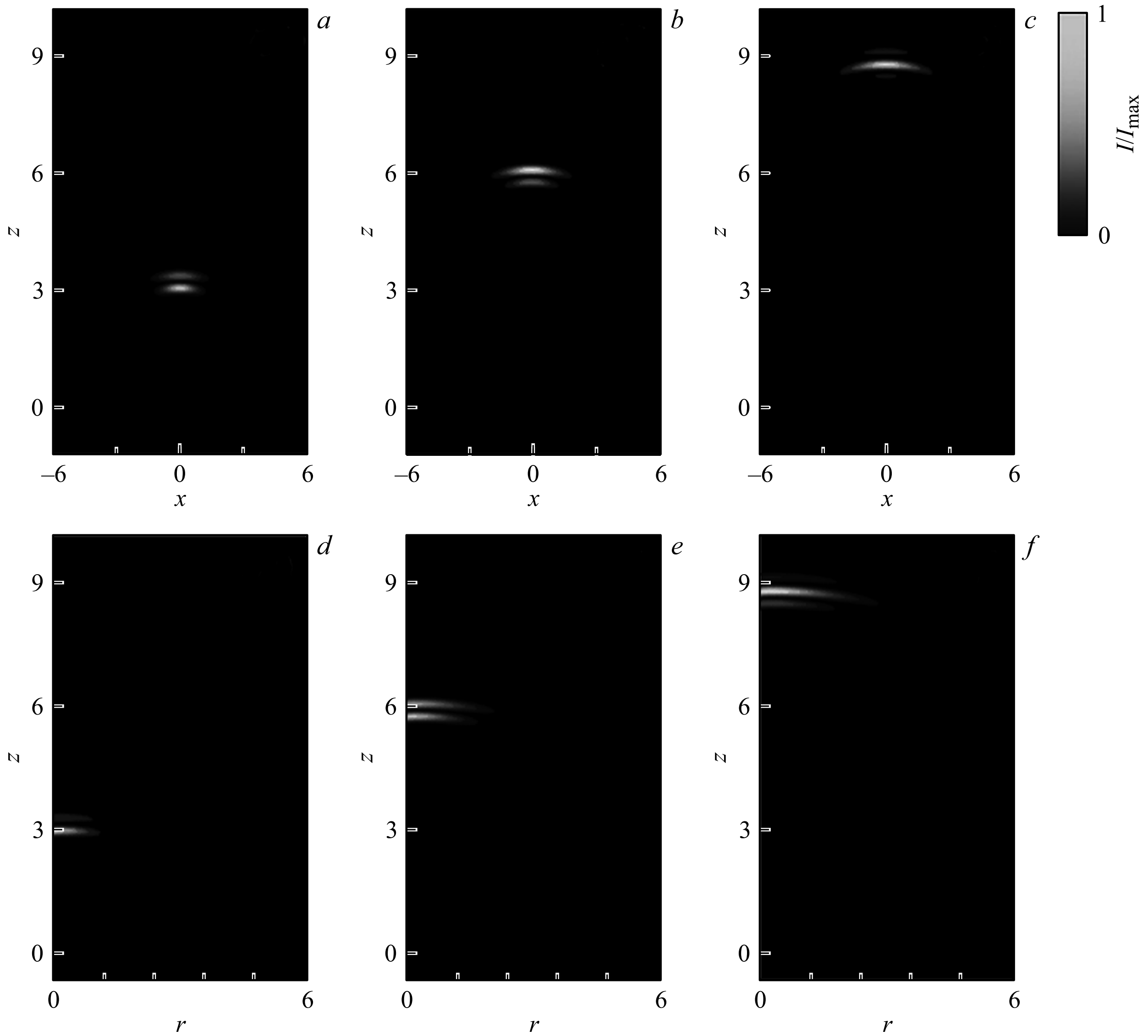

Figure 1. Dependence of the pulse intensity on the coordinates in the $2D(a-c)$- and $3D(d-f)$-cases at different points of time: (a, d) $t = 3.5$, (b, e) $t = 6.5$, (c,f) $t = 9.5$ Time unit corresponds to $3 \cdot 10^{-13}$ s, coordinate unit (z and r) — 10^{-3} cm. $I_{\max}$ — maximum intensity (separately for $2D$- and $3D$-cases).

follows

$$\frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} - \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial A}{\partial r}\right) - \frac{\partial^2 A}{\partial r}\frac{\partial^2 A}{\partial \phi^2} = -\mu\frac{\partial\langle S\rangle}{\partial t} + \frac{4\pi}{c}j(A), \qquad (4)$$

r, z, φ are coordinates in cylindrical system.

Let us write down further the law of dispersion of electrons in CNT [15], which will allow us to determine the electric current arising in CNT:

$$\varepsilon_s(p) = \pm\gamma_0\sqrt{1 + 4\cos\left(\frac{ap}{\hbar}\right)\cos\left(\frac{\pi s}{m}\right) + 4\cos^2\left(\frac{\pi s}{m}\right)}, \qquad (5)$$

where $s = 1, 2, \ldots, m$, nanotube is of type $(m, 0)$, $\gamma_0 \approx 2.7$ eV, $a = 3b/2$, b is the distance between adjacent carbon atoms.

The electric current density along the CNT axis can be calculated [9] by the formula

$$j = 2e\sum_{s=1}^{m}\int_{-\pi\hbar/a}^{\pi\hbar/a} v(ps)f(p,s)dp, \qquad (6)$$

where e is electron charge, p is electron quasi-momentum component, v_{ps} is electron speed, $f(p, s)$ is Fermi distribution function .

The angle derivative can be set equal to zero due to the cylindrical symmetry and the smallness of the accumulated charge [16]. In this case, equations (3) and (4) will be as

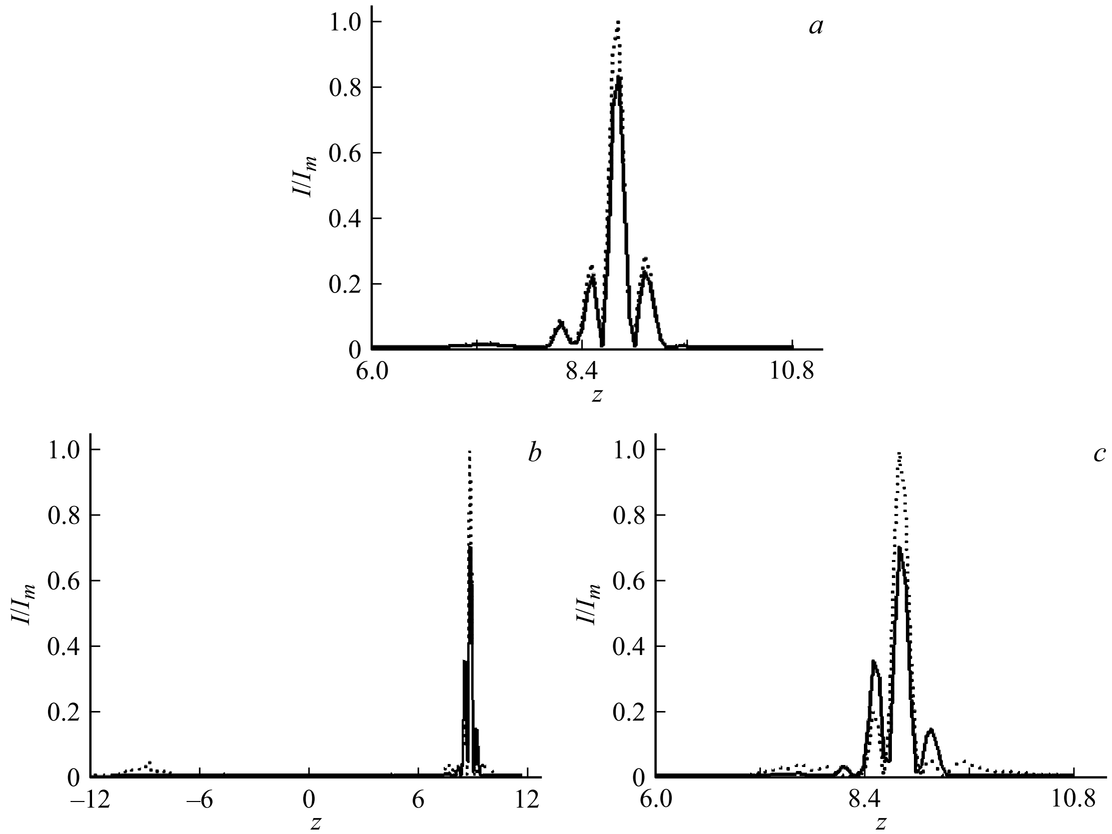

Figure 2. Dependence of the intensity of the electric field of the pulse on the coordinates at different temperatures (longitudinal sections at $t = 9.5$). (*a*) 2*D*-case, (*b, c*) 3*D*-case, solid curve is $T = 123$ K, dotted curve is $T = 56$ K Unit by coordinate z 10^{-3} cm. I_m is maximum intensity value for each picture separately.

follows

$$\nabla^2 A + \frac{4\pi e\sigma\gamma_0 a}{c\hbar}\sum_{q=1}^{\infty} b_q \sin\left(q\frac{aeA}{c}\right) - \mu\frac{\partial\langle S\rangle}{\partial t} = \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2}, \tag{7}$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial A}{\partial r}\right) + \frac{\partial^2 A}{\partial z^2} + \frac{4\pi e\sigma\gamma_0 a}{c\hbar} \times \sum_{q=1}^{\infty} b_q \sin\left(a\frac{aeA}{c}\right) - \mu\frac{\partial\langle S\rangle}{\partial t} = \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2}, \tag{8}$$

σ — concentration of electrons,

$$b_q = -\frac{q}{\gamma_0} \times \frac{\sum_s a_{s,q} \int\limits_{-\pi\hbar/a}^{\pi\hbar a} \cos\left(q\frac{ap}{\hbar}\right)\left(1+\exp\left(\sum_{q=1}^{\infty}\frac{a_{s,q}}{k_B T}\cos\left(q\frac{ap}{\hbar}\right)\right)\right)^{-1} dp}{\sum_s \int\limits_{-\pi\hbar/a}^{\pi\hbar a}\left(1+\exp\left(\sum_{q=1}^{\infty}\frac{a_{s,q}}{k_B T}\cos\left(q\frac{ap}{\hbar}\right)\right)\right)^{-1} dp}, \tag{9}$$

$a_{s,q}$ are coefficients of the Fourier expansion of the dispersion law (5).

Note that as the number q increases, there is a significant decrease in the coefficients b_q defined by formula (9). This allows us to consider only the first 10 terms.

The system of equations (1) and (7) (or (8) in the three-dimensional case) was reduced to a dimensionless form and solved numerically. The initial conditions for the pseudospin (10), as well as for the vector potential for two-dimensional (11) and three-dimensional problems (12) have the following form:

$$S = S_0, \qquad \beta = \frac{\operatorname{arth}(2S_0)}{JS_0}, \tag{10}$$

$$A = Q\exp\left(-\frac{z^2}{l_z^2}\right)\exp\left(-\frac{x^2}{l_x^2}\right),$$

$$\frac{dA}{dt} = \frac{2uQ}{l_z^2}\exp\left(-\frac{z^2}{l_z^2}\right)\exp\left(-\frac{x^2}{l_x^2}\right), \tag{11}$$

$$A = Q\exp\left(-\frac{z^2}{l_z^2}\right)\exp\left(-\frac{r^2}{l_r^2}\right),$$

$$\frac{dA}{dt} = \frac{2uQ}{l_z^2}\exp\left(-\frac{z^2}{l_z^2}\right)\exp\left(-\frac{r^2}{l_r^2}\right), \tag{12}$$

where Q is the amplitude of the electromagnetic pulse at the entrance to the medium with CNTs, l_i

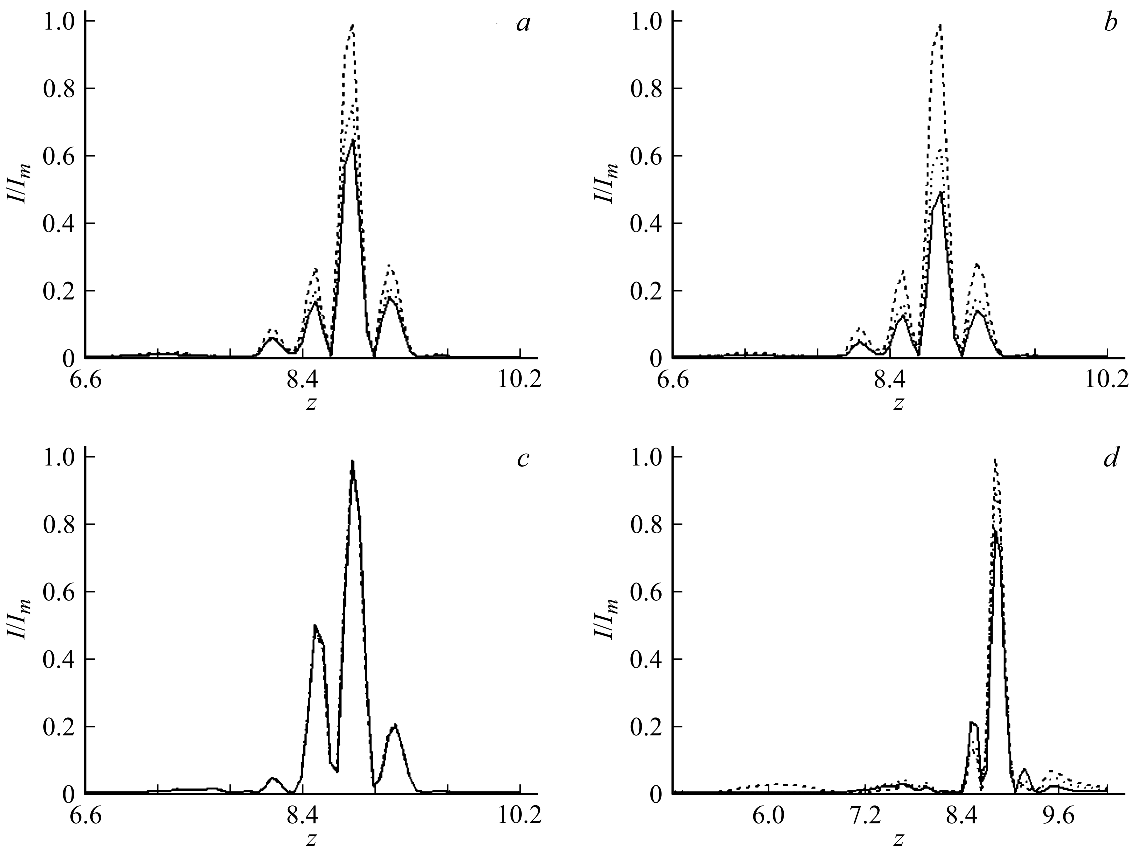

Figure 3. Dependence of the intensity of the electric field of the pulse on the coordinates for different values of the parameter μ (longitudinal sections at $t = 9.5$). (a, b) $2D$-case, (c, d) $3D$-case, solid curve is $\mu = 0.0125$, broken curve is $\mu = 0.025$, dashed curve is $\mu = 0.05$. Pictures (a, c) correspond to $T = 123\,\mathrm{K}$; (b, d) $T = 56\,\mathrm{K}$ Unit by coordinate z 10^{-3} cm. I_m is maximum intensity value for each picture separately.

$(i = x, y, z, r)$ determine the pulse width along the i-th direction, u is initial pulse velocity along the propagation axis, S_0 is pseudospin value at the initial moment of time, which allows determining the temperature at $t = 0$.

Simulation results

As shown by the results of the performed calculations, the second and third terms in the argument of the hyperbolic tangent from equation (1) do not affect the pulse dynamics, so we do not take them into account in what follows. The emerging evolution of the electric field of the pulse for the two-dimensional and three-dimensional cases is shown in Fig. 1. Note that the intensity is determined by the formula $I = c^{-2}(\partial A/\partial t)^2$.

Figure 1 demonstrates the steady propagation of the pulse in both cases.

The effect of temperature on the optical pulse in a ferroelectric medium with CNTs is shown in Fig. 2.

Fig. 2, *b* shows the range from -12 to 12 units to demonstrate the „tail" that follows the main pulse at $T = 56\,\mathrm{K}$. Figure 2, *c* is constructed in the same interval as Fig. 2, *a* to visualize the effect of temperature. It can be seen that in the three-dimensional case, the phase transition has a stronger effect on the shape and amplitude of the pulse.

The effect of the μ parameter on the shape of an extremely short optical pulse is shown in Fig. 3.

The parameter μ allows one to control the pulse amplitude in the two-dimensional case at a temperature corresponding to two phase states. In the three-dimensional case, for $T = 56\,\mathrm{K}$, the behavior is similar; for $T = 123\,\mathrm{K}$, no changes are observed for different values μ.

We also studied the behavior of the momentum as a function of the dipole moment δ. It is found that in the $2D$-case, an increase in the δ parameter leads to an increase in the pulse, in the $3D$-case, its influence is extremely small and manifests itself mainly in an increase in the „tail".

Conclusion

The following conclusions can be made according to the research results.

1. A system of effective equations has been obtained that describes the evolution of an extremely short pulse

in a ferroelectric medium with CNTs in the framework of Glauber's approach.

2. Simulation of the pulse dynamics in an impurity two-level system has been carried out in two-dimensional and three-dimensional cases.

3. The possibility of controlling the spatial characteristics of the pulse (shape and amplitude) by changing the temperature is demonstrated.

4. The shape of the pulse also depends on the dipole moment of the impurity pseudospin system.

5. The results obtained make it possible to use spectroscopy using extremely short pulses to reveal phase transitions due to impurities.

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Conflict of interest

The authors declare that they have no conflict of interest.

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