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NONLINEAR
AND QUANTUM OPTICS

Three-Dimensional Dissipative Quasi-Solitons in Carbon Nanotubes

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Abstract—The propagation of three-dimensional quasi-solitons in a system of carbon nanotubes with two-level impurities has been investigated. The system of effective equations is derived in the form of analogs of the Sine–Gordon classical equation and Bloch equations. The effects observed with a change in the inverse population and damping parameter have been studied.

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The generalization of the existing soliton models, aimed at making them closer to real physics, mainly by taking into account dissipation (an integral part of any system), has been one trend of study of solitons as nonlinear stable formations [1, 2]. Recently, much attention has been paid to the theory of dissipative solitons [3–5], which is one of these generalizations. These structures have been found in various systems, such as semiconductor optical amplifiers, laser systems with saturable absorption, magnetooptics, etc. [6, 7]. The stability of solitons, which is determined by the balance between dispersion and nonlinearity, is supplemented with the condition of balance between the arriving and dissipated energy flows.

At the same time, carbon nanotubes (CNTs) are widely known to have unique nonlinear properties, which suggest the existence of conventional solitons therein [8–10]. For example, nonlinear properties of CNTs with impurities were investigated within the Anderson periodic model [11]. The problems of nonlinear response of CNTs to a high-frequency electric field were considered in [12]. As was concluded in those studies, nonlinearity arises due to the change in the classical electron-distribution function and the nonparabolic electron-dispersion relation. The possibility of solitons existing in CNTs was established and the influence of CNT parameters on them was determined in [13, 14]. Therefore, the question of the existence of dissipative solitons in these systems (including three-dimensional ones) is quite natural [15]. Due to the existence of natural energy dissipation caused by scattering of CNT electrons from inhomogeneities and impurities, it is necessary to suggest a means of energy “pumping.” To solve this problem, we will supplement CNTs with two-level systems in the inverted state, which serve as “pump” ones.

CNTs and two-level systems with simple and thoroughly investigated model Hamiltonians were chosen as objects of microscopic consideration.

MAIN EQUATIONS AND RESULTS

Let us consider the propagation of three-dimensional ultrashort electromagnetic pulses in an array of zigzag CNTs.

The dispersion relation describing the properties of zigzag CNTs can be written as [16]

$$\varepsilon_s(p) = \pm\gamma\sqrt{1 + 4\cos(ap_z)\cos(\pi s/n) + 4\cos^2(\pi s/n)}, \qquad (1)$$

where $\gamma \approx 2.7$ eV, $a = 3b/2\hbar$ nm, and $b = 0.142$ nm is the distance between neighboring carbon atoms with a quasi-momentum (p_z, s) (p_z is the momentum component along the CNT axis, $s = 0, \ldots, n$). Different signs denote the valence and conduction bands.

It follows from the quantum mechanics laws that, in the presence of external electric field $\mathbf{E}$ (directed for clarity along the x axis and considered below in the calibration $E = -\partial A/c\partial t$), the momentum must be replaced by generalized momentum $\mathbf{p} \to \mathbf{p} - e\mathbf{A}/c$ (e is the elementary charge).

The three-dimensional wave equation for the electric-field vector potential in the cylindrical coordinate system can be written as

$$A_{tt} + \frac{4\pi\mu n}{c^2} P_t + \Gamma A_t = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial A}{\partial r}\right) + \frac{\partial^2 A}{\partial z^2} + \frac{1}{r^2}\frac{\partial^2 A}{\partial \varphi^2} + 4\pi j(A), \quad (2)$$

where $P = 2\mu\langle\sigma^z\rangle$, μ is the effective electric-dipole moment of one two-level system of the sample, and $\langle\sigma^z\rangle$ is the mean value of the z component of the pseudospin vector. Here, we passed to the continuum limit and introduced concentration n of two-level systems (c is the speed of light, and Γ is the damping parameter). A transition to the continuum limit should also be made in the Heisenberg equations of motion for the mean values of pseudospin operators of two-level systems, which are uncoupled within the random-phase approximation. The fact that the characteristic spatial size of their localization is much higher than the distance between neighboring two-level systems even for femtosecond pulses should also be taken into account. Then, as was noted in [17, 18], one can easily obtain

$$\frac{d\langle\sigma^x\rangle}{dt} = -2\frac{\mu}{c}\frac{\partial A}{\partial t}\langle\sigma^y\rangle,$$
$$\frac{d\langle\sigma^y\rangle}{dt} = \Omega\langle\sigma^z\rangle + 2\frac{\mu}{c}\frac{\partial A}{\partial t}\langle\sigma^x\rangle, \quad (3)$$
$$\frac{d\langle\sigma^z\rangle}{dt} = -\Omega\langle\sigma^y\rangle,$$

where Ω describes the transitions in a two-level system.

Note that dynamics equations of two-level centers (3) do not contain relaxation parameters (i.e., they are valid only for times much shorter than the relaxation time). Since we are considering ultrashort pulses (USPs), the relaxation processes can be neglected.

Due to the cylindrical symmetry, it is assumed below that $\frac{\partial}{\partial\varphi} \to 0$. This assumption should be additionally discussed. Due to the field nonuniformity along some axis (we assume for clarity that the field is directed along the x axis and is nonuniform in this direction), the current is also nonuniform. The current nonuniformity causes charge accumulation in some region. The accumulated charge can most easily be estimated from the charge-conservation law:

$$\frac{d\rho}{dt} + \frac{dj}{dx} = 0, \quad (4)$$

$$\rho \propto \tau\frac{j}{l_x}. \quad (5)$$

Here, ρ is the charge density, j is the current density along the x axis, τ is the electric-field pulse width, and l_x is the characteristic length at which the pulse electric field changes along the x axis.

It follows from (5) that the USP width affects significantly the accumulated charge, which induces an additional electric field to interfere the USP field. The accumulated charge was estimated to be about 1–2% of the charge contributing to the current; hence, the charge accumulation can be considered negligible for femtosecond pulses [19]. The numerical experiments for CNTs and a pulse width of several tens of femtoseconds confirm the validity of this assumption [19].

The standard expression for the current density can be written as

$$j = e\sum_p v_y\left(p - \frac{e}{c}A(x,t)\right)\langle a_p^+ a_p\rangle, \quad (6)$$

where $v_y(p) = \frac{\partial\varepsilon(p_x, p_y)}{\partial p_y}$ and the angle brackets indicate averaging with nonequilibrium density matrix $\rho(t)$: $\langle B\rangle = \mathrm{Tr}(B(0)\rho(t))$. With allowance for the equality $[a_p^+ a_p, H] = 0$, the equation of motion yields directly $\langle a_p^+ a_p\rangle = \langle a_p^+ a_p\rangle_0$ for the density matrix, where $\langle B\rangle_0 = \mathrm{Tr}(B(0)\rho(0))$. Thus, one can use the number of particles given by the Fermi–Dirac distribution in the expression for the current density. We consider below the case of low temperatures, in which only a small region in the pulse space near the Fermi level contributes to the sum (integral).

Taking into account that $\rho_0 = \exp(-H/kT)/\mathrm{Tr}(\exp(-H/kT))$ (k is the Boltzmann constant, and T is temperature), we expand $v_s(p)$ in a Fourier series:

$$v_s(p) = \sum_k A_{ks}\sin(kp),$$
$$A_{ks} = \frac{1}{2\pi}\sum_p v_s(p)\sin(kp).$$

Then,

$$v_s\left(p - \frac{e}{c}A(t)\right) = \sum_k A_{ks}\sin(kp)\cos\left(\frac{ke}{c}A(t)\right) - \cos(kp)\sin\left(\frac{ke}{c}A(t)\right)$$

and, taking into account that distribution function $\rho(0)$ is an even function of quasi-momentum, which turns to zero when averaging $\sin(kp)$, one can write

$$v_s\left(p - \frac{e}{c}A(t)\right) = -\sum_k A_{ks}\cos(kp)\sin\left(\frac{ke}{c}A(t)\right). \quad (7)$$

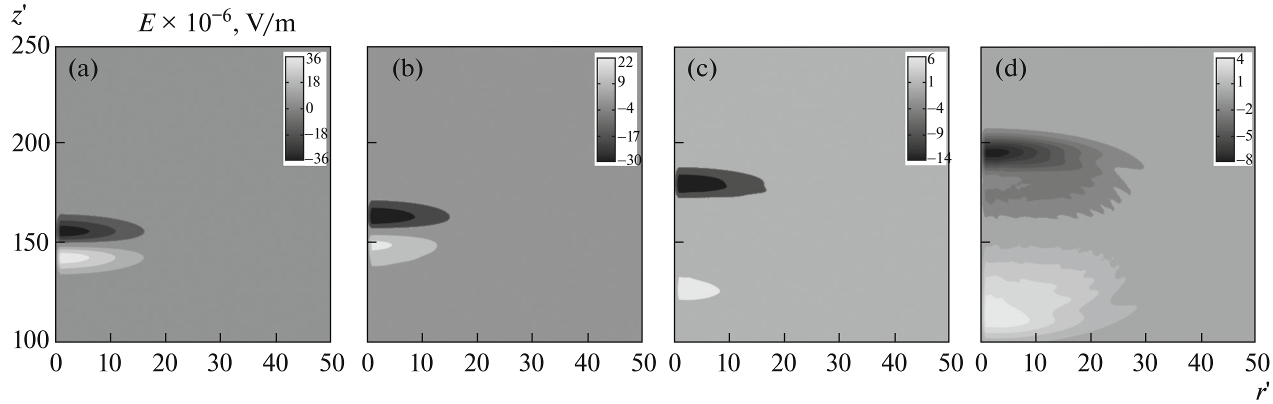

Fig. 1. Strength of the electric field of a three-dimensional electromagnetic pulse at different instants: (a) initial instant and t = (b) 1.0×10^{-13}, (c) 3.0×10^{-13}, and (d) 5.0×10^{-13} s.

Substituting this result into (6) and performing summation over s and p, we obtain

$$j = -en_0 \sum_k f_k \sin\left(\frac{ke}{c} A(t)\right),$$

$$f_k = \sum_{s=1}^{m} \int_{-\pi/a}^{\pi/a} dp A_{ks} \cos(kp) \frac{\exp(-\beta\varepsilon_s(p))}{1 + \exp(-\beta\varepsilon_s(p))},$$

where n_0 is the concentration of equilibrium electrons in the system and $\beta = 1/kT$.

Taking into account all the aforesaid and introducing dimensionless values, we can write Eq. (2) as

$$B_{t't'} = \frac{1}{r'}\frac{\partial}{\partial r'}\left(r'\frac{\partial B}{\partial r'}\right) + \frac{\partial^2 B}{\partial z'^2} + \frac{1}{r'^2}\frac{\partial^2 B}{\partial \varphi'^2}$$
$$+ \sin(B) + \sum_{k=2}^{\infty} f_k \sin(kB) - \langle \sigma^y \rangle - \Gamma B_{t'}, \quad (8)$$
$$B = \frac{eaA}{c}, \quad t' = t\frac{ea}{c}\sqrt{8\pi n_0 \gamma |f_1|},$$
$$\varphi' = \varphi\sqrt{8\pi\gamma}, \quad r' = r\sqrt{8\pi\gamma}, \quad z' = z\sqrt{8\pi\gamma}.$$

Note that Eq. (8) is only a generalization of the well-known Sine–Gordon equation for the case in which the generalized potential is expanded in the general Fourier series.

Equations (3) and (8) were numerically solved [20]. The initial conditions were chosen in the form

$$B(z', r', 0) = Q\exp\left(-\frac{(z' - z_0)^2}{\gamma_z}\right)\exp\left(-\frac{r'^2}{\gamma_r}\right),$$
$$\frac{dB(z', r', 0)}{dt'} = 2Q\frac{z' - z_0}{\gamma_z}$$
$$\times \exp\left(-\frac{(z' - z_0)^2}{\gamma_z}\right)\exp\left(-\frac{r'^2}{\gamma_r}\right), \quad (9)$$
$$\left\langle \sigma^x \right\rangle\Big|_{t'=0} = -w, \quad \left\langle \sigma^y \right\rangle\Big|_{t'=0} = 0, \quad \left\langle \sigma^z \right\rangle\Big|_{t'=0} = 0,$$

where r' is the radius, Q is the amplitude, γ_z and γ_r determine the pulse width, z_0 is the initial displacement of the pulse center, and w is the inverse population. This initial condition corresponds to the case in which a USP consisting of one electric-field oscillation is applied to the sample. The energetic parameters were expressed in Δ units. Note that the evolution variable in this consideration is time.

The evolution of the electromagnetic field propagating over the sample is shown in Fig. 1.

The USP is split into two pulses with amplitude loss, and these pulses begin to propagate separately. In turn, each pulse formed from the initial one is also split into two pulses during propagation, etc. One can relate this process to the removal of inverse population from two-level systems during their propagation. Similar behavior (splitting of the initial pulse and further propagation) was observed when investigating the USP dynamics in nanotube systems [13, 14].

Here, the use of the term "soliton" is extremely conventional, because pulses undergo splitting. Therefore, we will use another term: "quasi-soliton."

The influence of damping parameter Γ is shown in Fig. 2. It can be seen that the Γ value significantly affects the USP shape. An increase in Γ leads to an increase in the number of pulses the main pulse is split into (although case (b) with $\Gamma = 2$ is inconsistent with the general pattern).

An important distinctive feature of dissipative quasi-solitons is that their shape depends weakly on the initial conditions. The dependence of the pulse shape on the inverse population w, which is related to the initial distribution, was investigated in the system under consideration to confirm the existence of this feature (Fig. 3).

It can be seen in Fig. 3 that the pulses corresponding to different initial conditions begin to acquire an identical shape as they recede from the pulse-location point at the initial instant and the difference between them decreases. This fact, in turn, suggests that the

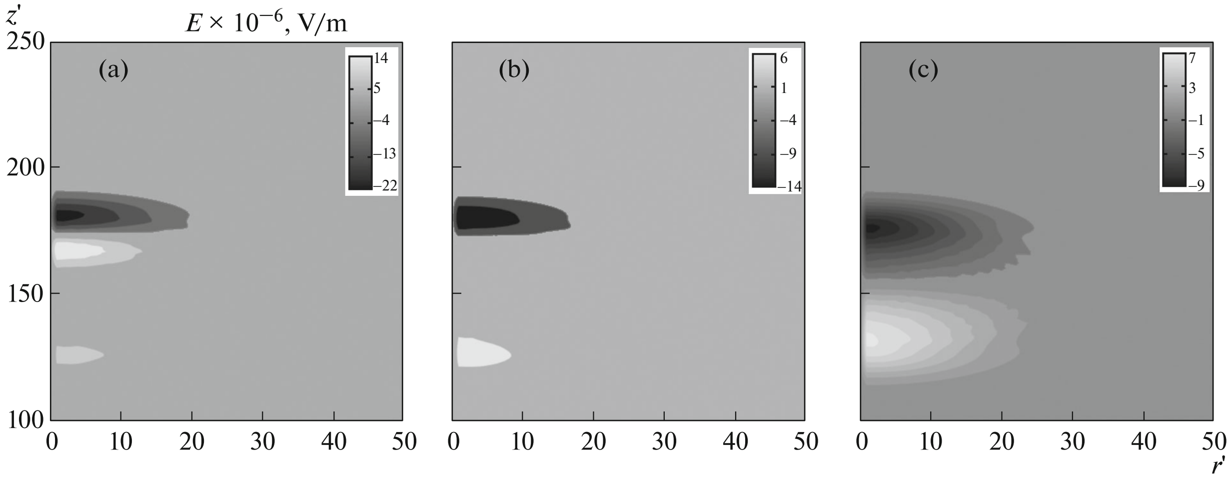

Fig. 2. Strength of the electric field of a three-dimensional electromagnetic pulse for $w = 2$; $t = 3.0 \times 10^{-13}$ s; and Γ = (a) 1.0, (b) 2.0, and (c) 4.0 rel. units.

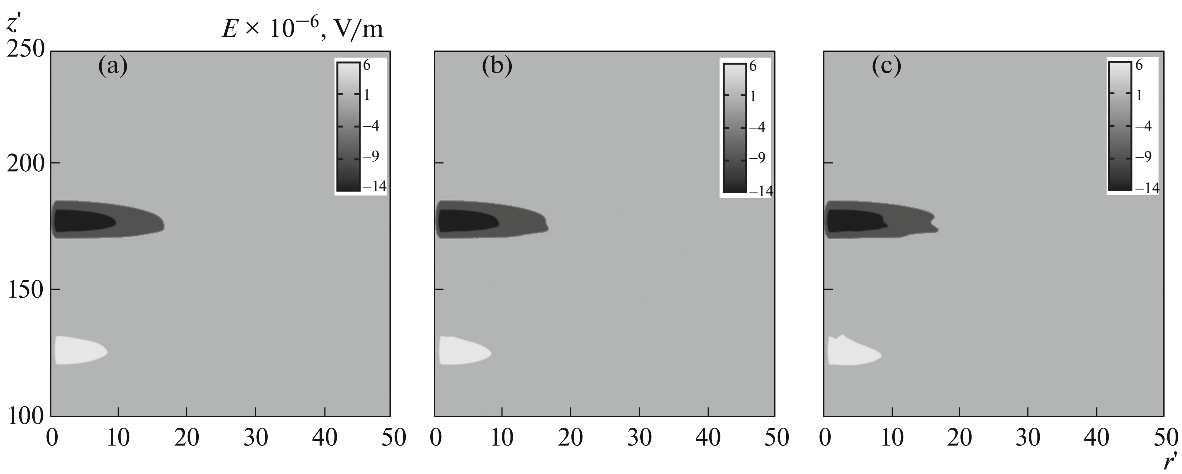

Fig. 3. Strength of the electric field of a three-dimensional electromagnetic pulse for $\Gamma = 2$; $t = 3.0 \times 10^{-13}$ s; and w = (a) 1.0, (b) 2.0, and (c) 4.0 rel. units.

specific features observed in the system under consideration are the same as in the case of the formation of dissipative solitons.

CONCLUSIONS

The conclusions based on the results of this study can be formulated as follows.

(i) An ultrashort optical pulse propagates without amplitude damping, which is due to the balance between its energy loss and the energy takeoff from inverted two-level systems.

(ii) The propagation of an ultrashort optical pulse causes a "tail" of electric-field oscillations behind it, which can be explained as being due to excitation of nonlinear-wave pulses.

(iii) The shape of the arising pulse train (i.e., electric-field peaks, which are constantly split into similar peaks) at large distances depends weakly on the initial conditions due to the dissipation and gain in this system.

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