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Extremely short optical pulse in a system of nanotubes with adsorbed hydrogen

Mikhail B. Belonenko [a], Alexander S. Popov [b], Nikolay G. Lebedev [b], Anastasia V. Pak [b], Alexander V. Zhukov [c,d,*]

[a] Volgograd Institute of Business, 400048 Volgograd, Russia
[b] Volgograd State University, 400062 Volgograd, Russia
[c] Institute for Cancer Research and Treatment, 10060 Candiolo, Torino, Italy
[d] M_2NeT Lab, Wilfrid Laurier University, Waterloo, ON, N2L 3C5, Canada

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ABSTRACT

In this Letter we address the system of carbon nanotubes with adsorbed hydrogen, which is a problem of particular practical importance. Based on the periodic Anderson model we describe the electronic subsystem in such a system, so that employing the method of Green functions allowed us to obtain the dispersion law for electrons. In the low-temperature limit we investigated a joint dynamics of electrons and electromagnetic field. The effective equation, which describes the propagation of ultrashort optical pulses, has been derived. We analyze the solutions of this equation and their dependence on the parameters of the problem for a two-dimensional CNT system.

1. Introduction

Recent boom of interest in nonlinear phenomena significantly stimulated the creation of materials that can exhibit nonlinear properties under readily accessible experimental conditions. Among such materials there are carbon nanotubes, which represent a structure that consists of a single layer of carbon atoms arranged in a hexagonal lattice, rolled into a cylinder. High mobility of electrons in carbon nanotubes and their unique electrical characteristics attract an attention to them, as to a possible alternative to the silicon base of the modern microelectronics [1–4]. Although usually the dispersion of electrons in carbon nanotubes is chosen from the imposition of periodic boundary conditions on the dispersion relation in graphene it should be noted that carbon nanotubes can easily adsorb various impurities and, as a result, a proper account of the interaction within electronic system of nanotubes becomes a difficult task [5,6]. In particular, the interaction of electrons of nanotubes and impurity electrons can lead to a qualitative change in the energy spectrum (for example, the formation of a gap in the spectrum), and therefore propagation of optical pulses becomes possible. We would also like to note that in the situation described above the energy spectrum of electrons in the minibands is strongly nonparabolic. This in turn leads to the fact that the nonlinearity of the electronic properties of carbon nanotubes can be visible even in fields of moderate intensity [7,8]. Based on this, we can formulate the main objective of the work as the study of propagation of optical pulses of short duration through an array of carbon nanotubes.

Note that, apparently, the easiest way to take into account the interaction of nanotube electrons and impurity electrons is the one proposed by Anderson [9,10], when only the hybridization of electronic subsystems is taken into account. Modification of the dispersion law of elementary excitations in the Anderson impurity model is well known, and therefore the problem appears on how to consistently account for this change in the optical response of matter.

Since carbon nanotubes, subject to the geometric configuration, can have conducting properties, then this model is well justified for the description of the adsorption in a system under consideration. Periodic Anderson model deals with the two groups of electrons: collective s-electrons and localized d-electrons.

Collective particles are free, while the localized particles interact with each other via the Coulomb repulsion on the site. In contrast to the *sd*-model, the interaction between *s*- and *d*-electrons occurs not due to exchange forces, but hybridization. In general, the periodic Anderson model is defined by the Hamiltonian

$$H = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \epsilon_d \sum_{i\sigma} n^d_{i\sigma} + U \sum_i n^d_{i\uparrow} n^d_{i\downarrow} + \sum_{ij\sigma} \left(V_{ij} c^{\dagger}_{i\sigma} d_{j\sigma} + V^*_{ij} d^{\dagger}_{j\sigma} c_{i\sigma} \right), \quad (1)$$

where $c_{j\sigma}$ ($c^{\dagger}_{j\sigma}$) and $d_{j\sigma}$ ($d^{\dagger}_{j\sigma}$) are the Fermi-operators describing *s*- and *d*-electrons respectively, $n^d_{i\sigma} = d^{\dagger}_{i\sigma} d_{i\sigma}$ is the number of *d*-electrons with the spin σ at the ith site; ϵ_d is the energy level of *d*-electron at the site, and V_{ij} is the hybridization parameter.

* Corresponding author at: Institute for Cancer Research and Treatment, 10060 Candiolo, Torino, Italy.
E-mail address: alex.zhukov@gmail.com (A.V. Zhukov).

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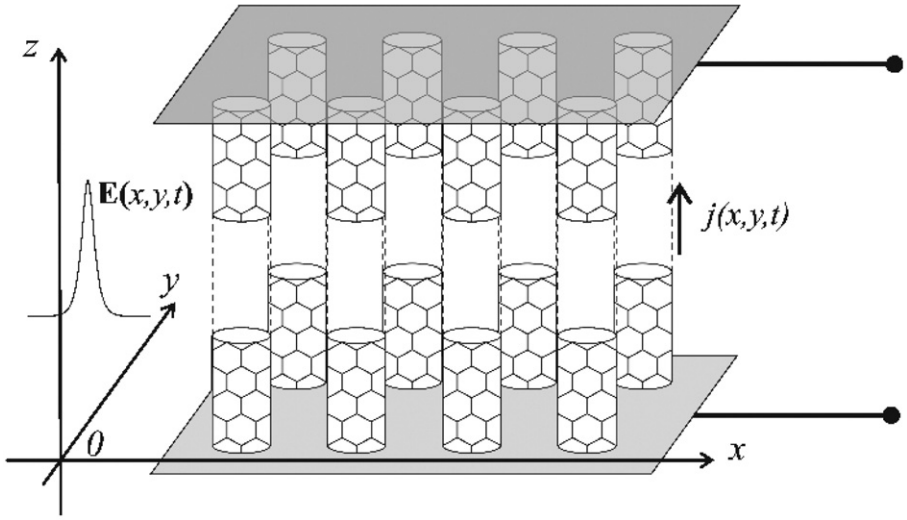

Fig. 1. Geometry of the problem. Ultrashort optical pulse with the electric field $\mathbf{E}(x,t)$, directed along the tube z-axis, moves in the transverse direction along the x-axis.

This model particularly describes the localized atomic moments, the Kondo insulators, heavy fermions, and intermediate valence. It is the second basic model for high-temperature superconductors [11].

In this work the atomic hydrogen and alkali metal atoms are considered as impurities adsorbed on the surface of carbon nanotubes.

2. The model

Consider an extremely short optical pulse propagating in a two-dimensional array of carbon nanotubes. As usual, using the notion "extremely short optical pulses" we mean a pulse which consists of a small number of electromagnetic field oscillations. Such a pulse has an area of spatial localization which is comparable with the wavelength and it cannot be divided into the "envelope" and "carrier" parts. Electric field vector $\mathbf{E}(x,y,t)$ is directed along the tube axis z, and an electromagnetic wave propagates in the transverse direction along the x-axis (Fig. 1).

Let us consider the sequence of packing layers of carbon nanotubes (with a zigzag structural modification) to be of the ideal ABAB-type with equal {0002} interlayer distance of about 0.34 nm [12]. The interaction between the CNTs is not considered, therefore a type of packing in an array is not important. For simplicity and definiteness, we assume that the unit cell contains four atoms and its group of spatial symmetry is P42/mmc (D94h) [12]. We have to note that the questions related to the presence of the substrate, on which nanotubes are grown, are beyond the scope of this article. In fact it means that we neglect the presence of surface waves, the effects of charge accumulation in the substrate and the appearance of an additional electric field directed along the nanotube axis. Perfect carbon nanotubes of "zig-zag" type are characterized by chiral indices $(n,0)$, where n actually determines the diameter of the tube. The electronic structure of such tubes is described by well-known dispersion relation obtained in the framework of π-electron Hückel approximation [12]

$$\epsilon(\mathbf{p}) = \pm\gamma\left\{1 + 4\cos(ap_z)\cos\left(\frac{\pi s}{n}\right) + 4\cos^2\left(\frac{\pi s}{n}\right)\right\}^{1/2}, \qquad (2)$$

where $\gamma \approx 2.7$ eV, $a = 3b/2\hbar$, $b = 0.142$ nm is the distance between adjacent carbon atoms. Quasi-momentum $\mathbf{p}$ has the components (p_z, s), where p_z is the component directed along the nanotube axis, while $s = 1, 2, \ldots, n$ is the number, which characterizes the quantization of momentum along the perimeter of the nanotube. Different signs in Eq. (2) refer to the conduction and valence bands respectively.

Hybridization energy $V = V_{ij}$ in the Anderson Hamiltonian (1) can be estimated from the quantum-chemical approaches, since it is determined by the integral over the overlap of wave functions of s-orbital (the hydrogen atom) and p_z-orbital (carbon atom):

$$V = \frac{1}{2}(\beta_H + \beta_C)S_{HC}, \qquad S_{HC} = \int \psi_{1s}(\mathbf{r})\psi_{2p_z}(\mathbf{r})\,d^3r,$$
$$\psi_{1s} = \frac{1}{\sqrt{\pi}}\left(\frac{z}{a_0}\right)^{3/2} e^{-\rho}, \quad \rho = \frac{zr}{a_0}, \qquad z(H) = 1,$$
$$\psi_{2p_z} = \frac{1}{4\sqrt{2\pi}}\left(\frac{z}{a_0}\right)^{3/2} \rho e^{-\rho/2}\cos\theta, \quad \rho = \frac{zr}{a_0},$$
$$z(C) = 6, \qquad (3)$$

where S_{HC} is the integral of wave functions overlap, β_H and β_C are the parameters of the semiempirical quantum-chemical method MNDO [13], $\beta_H = -6.99$ eV, $\beta_C = -7.93$ eV, a_0 is the Bohr radius, and z is the charge of an atom.

Estimates of the hybridization energy yield a value of $V = -1.43$ eV. This is the energy of an electron in a system of two nuclei. A bound state is formed in this case, so that the energy is negative.

When considering the adsorption of alkali metals we have taken into account only the overlap of the outer valence s-orbitals with the $2p_z$-orbital of carbon atom. The wave functions of valence electrons for lithium, sodium, and potassium are correspondingly given by [14]

$$\psi_{2s} = \frac{1}{4\sqrt{2\pi}}\left(\frac{z}{a_0}\right)^{3/2}(2-\rho)e^{-\rho/2}, \quad \rho = \frac{zr}{a_0},$$
$$\psi_{3s} = \frac{2}{81\sqrt{3\pi}}\left(\frac{z}{a_0}\right)^{3/2}(27 - 18\rho + 2\rho^2)e^{-\rho/3}, \quad \rho = \frac{zr}{a_0},$$
$$\psi_{4s} = \frac{1}{768\sqrt{4\pi}}\left(\frac{z}{a_0}\right)^{3/2}(192 - 144\rho + 24\rho^2 - \rho^3)e^{-\rho/4},$$
$$\rho = \frac{zr}{a_0}.$$

Hybridization potentials were calculated similarly to the hydrogen atom. The corresponding values of hopping integrals, computed using the semiempirical MNDO method are

$$\beta_{\mathrm{Li}} = -1.35\ \mathrm{eV}, \qquad \beta_{\mathrm{Na}} = -0.16\ \mathrm{eV}, \qquad \beta_{\mathrm{K}} = -3.53\ \mathrm{eV}.$$

Within the frame of the same semiempirical MNDO method the values of energy of the adatoms can be estimated as follows:

$$\epsilon_a^{(\mathrm{Li})} = -5.13\ \mathrm{eV}, \qquad \epsilon_a^{(\mathrm{Na})} = -5.14\ \mathrm{eV}, \qquad \epsilon_a^{(\mathrm{K})} = -4.34\ \mathrm{eV}.$$

Corresponding hybridization energies are given by

$$V_{\mathrm{Li}} = -1.45\ \mathrm{eV}, \qquad V_{\mathrm{Na}} = -0.07\ \mathrm{eV}, \qquad V_{\mathrm{K}} = -0.01\ \mathrm{eV}.$$

To estimate the energy of an adatom we use the method of images [15], based on the fact that the conductor is an equipotential surface [16]. As a result we obtain the following formula

$$\tilde{\epsilon}_a = I + \frac{1}{4\pi\varepsilon_0}\frac{e^2}{4l},$$

where $I = -13.6$ eV is the ionization potential of the hydrogen atom, e is the elementary charge, ε_0 is the electric constant, $l = 1.2$ Å is the distance from the center of the adatom to the plane of its image on the substrate. The latter is of the order of atomic radius of the adatom (the adsorption bond length), which was estimated from quantum-chemical semiempirical calculations [17].

To obtain the statistical correlation characteristics of the structures of interest we have used mathematical formalism of Green's functions [18] and the methodology explicitly described in [19]. This method is widely used in statistical mechanics due to the fact that it provides an effective tool for calculating the observable macroscopic characteristics of the system as well as the microscopic (e.g. the energy of elementary excitations and their lifetime). The equations of motion for the Fourier transforms of the single-particle Green's functions [19] of an adsorbed atom are as follows

$$\begin{aligned} E\langle\langle a_\lambda | a_\lambda^\dagger\rangle\rangle_E^r = {} & \frac{i}{2\pi}\langle [a_\lambda, a_\lambda^\dagger]_+\rangle + \sum_{k\sigma}\epsilon_k\langle\langle [a_\lambda, c_{k\sigma}c_{k\sigma}^\dagger]|a_\lambda^\dagger\rangle\rangle_E^r \\ & + \epsilon_a\sum_\sigma\langle\langle [a_\lambda, a_\sigma a_\sigma^\dagger]|a_\lambda^\dagger\rangle\rangle_E^r \\ & + \sum_{k\sigma}V_{ka}\langle\langle [a_\lambda, c_{k\sigma}^\dagger a_\sigma]|a_\lambda^\dagger\rangle\rangle_E^r \\ & + \sum_{k\sigma}V_{ka}^*\langle\langle [a_\lambda, a_\sigma^\dagger c_{k\sigma}]|a_\lambda^\dagger\rangle\rangle_E^r. \end{aligned}$$

After calculating the commutators, the above equation is transformed to (ω is the energy variable)

$$\omega\langle\langle a_\lambda | a_\lambda^\dagger\rangle\rangle_\omega^r = \frac{i}{2\pi} + \epsilon_a\langle\langle a_\lambda | a_\lambda^\dagger\rangle\rangle_\omega^r + \sum_k V_{ka}^*\langle\langle c_{k\lambda} | a_\lambda^\dagger\rangle\rangle_\omega^r.$$

The equations for the Green's function of the crystal have the form

$$\begin{aligned} E\langle\langle c_{l\nu} | c_{l\nu}^\dagger\rangle\rangle_E^r = {} & \frac{i}{2\pi}\langle [c_{l\nu}, c_{l\nu}^\dagger]_+\rangle + \sum_{k\sigma}\epsilon_k\langle\langle [c_{l\nu}, c_{k\sigma}c_{k\sigma}^\dagger]|c_{l\nu}^\dagger\rangle\rangle_E^r \\ & + \epsilon_a\sum_\sigma\langle\langle [c_{l\nu}, a_\sigma a_\sigma^\dagger]|c_{l\nu}^\dagger\rangle\rangle_E^r \\ & + \sum_{k\sigma}V_{ka}\langle\langle [c_{l\nu}, c_{k\sigma}^\dagger a_\sigma]|c_{l\nu}^\dagger\rangle\rangle_E^r \\ & + \sum_{k\sigma}V_{ka}^*\langle\langle [c_{l\nu}, a_\sigma^\dagger c_{k\sigma}]|c_{l\nu}^\dagger\rangle\rangle_E^r. \end{aligned}$$

Analogously, we have

$$\omega\langle\langle c_{l\nu} | c_{l\nu}^\dagger\rangle\rangle_\omega^r = \frac{i}{2\pi} + \epsilon_l\langle\langle c_{k\sigma} | a_{l\nu}^\dagger\rangle\rangle_\omega^r + V_{la}\langle\langle a_\sigma | c_{l\nu}^\dagger\rangle\rangle_\omega^r.$$

As a result, an expression for the Green's function of the crystal lattice with the presence of a single defect atom of can be written as

$$\langle\langle c_{k\sigma} | c_{k\sigma}^\dagger\rangle\rangle = \frac{i}{2\pi}\frac{\omega - \epsilon_a}{(\omega - \epsilon_a)(\omega - \epsilon_k) - |V_{ka}|^2}. \tag{4}$$

Analytical expression for the Green's function of carbon nanotubes (4) allows us to determine the eigenvalues of the energies of elementary excitations in the crystal, appeared due to an adsorption of atomic hydrogen and alkali metal atoms. The energy eigenvalues of carbon nanotubes with attached defect atoms are given by the poles of Green's functions [19]. From formula (4) we can easily obtain an expression for the band structure of CNTs modified by adsorption of hydrogen atom, namely

$$E(p) = \frac{1}{2}\left\{\epsilon_a + \epsilon_p \pm \sqrt{(\epsilon_a - \epsilon_p)^2 + 4|V_{ka}|^2}\right\}, \tag{5}$$

where ϵ_p is the band structure of an ideal carbon nanotube, which has the form (2).

In the 1D case, the evolution of the electromagnetic field of a pulse can be classically described on the basis of Maxwell equations [20]. Maxwell equations for the vector potential $\mathbf{A} = \{0, 0, A_z(x,t)\}$ for the 2D problem with the gauge $\mathbf{E} = -\partial\mathbf{A}/c\partial t$ can be presented in the form

$$\frac{\partial^2\mathbf{A}}{\partial x^2} - \frac{1}{c}\frac{\partial^2\mathbf{A}}{\partial t^2} = \frac{4\pi}{c}\mathbf{j}, \tag{6}$$

where we did not take into account the diffractive beam spreading in zth direction.

Using the semiclassical approximation, let us find the current density that is present implicitly in Eq. (5). In this approximation, the evolution of an ensemble of Fermi particles is described by the classical Boltzmann kinetic equation in the model of relaxation times [21]

$$\frac{\partial f}{\partial t} - \frac{q}{c}\frac{\partial A_z}{\partial t}\frac{\partial f}{\partial p_z} = \frac{F_0 - f}{\tau}. \tag{7}$$

Here the distribution function $f = f(p_z, s, t)$ implicitly depends on the spatial coordinates x and y via the vector potential, F_0 is the equilibrium Fermi function

$$F_0 = \frac{1}{1 + \exp(E(\mathbf{p})/k_B T)}, \tag{8}$$

T is the equilibrium temperature, k_B is the Boltzmann constant. The relaxation time τ can be estimated as $\sim 3\cdot 10^{-13}$ s [22].

Eq. (7) can be solved by the method of characteristics [23]. The result is

$$\begin{aligned} f = {} & F_0\left(p_z + \frac{q}{c}A_z(t)\right)e^{-t/\tau} \\ & + \frac{1}{\tau}\int_{-\infty}^{t} e^{-(t-t')/\tau}F_0\left(p_z + \frac{q}{c}\big(A_z(t) - A_z(t')\big)\right)dt'. \end{aligned} \tag{9}$$

Current density $\mathbf{j} = (0, 0, j_z)$ can be expressed in the frame of semiclassical approximation as

$$j_z = \frac{q}{\pi\hbar}\sum_s\int dp_z\, v_z f, \tag{10}$$

where $v_z = \partial E(\mathbf{p})/\partial p_z$ is the electron velocity, q is the elementary electric charge.

Note that Eq. (7) is neglecting the effects related to the heterogeneity of the electromagnetic field along the nanotube axis z. This is justified on the one hand by the assumption of a flat nature of the wavefront of the laser pulse, and on the other hand by

nanometer sizes of particles, which involve the implementation of this approach with the required accuracy. Assuming that the time scale in the system is large compared with the relaxation time τ, we neglect the first term in Eq. (9) and change the variables of integration $p \to p - e(A_z(t) - A_z(t'))/c$. Then the expression for the current density takes the following form:

$$j_z = \frac{q}{\pi\hbar\tau}\sum_s \int_{-\infty}^{t}\int_{-q_0}^{q_0} dt'\,dp_z\, v_z\left(s, p - \frac{q}{c}\big(A_z(t) - A_z(t')\big)\right) \times F_0(\mathbf{p}) e^{-(t-t')/\tau}, \tag{11}$$

where the integration is performed over the first Brillouin zone, and $q_0 = 2\pi\hbar/3b$ is the momentum at the Brillouin zone boundary.

Velocity component $v_z(s,p)$ can be expanded into a Fourier series

$$v_z(s,p) = \sum_m a_{ms}\sin(mp),$$
$$a_{ms} = \frac{1}{\pi}\int_{-\pi}^{\pi} v_z(s,p)\sin(mp)\,dp, \tag{12}$$

so that the current density looks

$$j_z = \frac{q}{\pi\hbar\tau}\sum_{ms} a_{ms}\int_{-\infty}^{t} dt'\,\sin\left(\frac{maq}{c}\big(A_z(t) - A_z(t')\big)\right)e^{-(t-t')/\tau} \times \int_{-q_0}^{q_0} dp_z\,\cos(map_z)F_0(\mathbf{p}). \tag{13}$$

Let us transform the integral containing the temporal exponent using the method, which is well known in the theory of semiconductor superlattices [24]. Making the substitution $\rho = t - t'$ and seeking for a solution for $A_z(t)$ belong a class of rapidly decreasing functions, let us take into account that the relaxation time τ is rather large as compared to the typical ultra-short laser pulses duration. This lead us to a conclusion that $A_z(t-\rho) \approx A_z(-\infty) = 0$. As a result of these transformations we finally come to the following equation for the vector potential:

$$\frac{\partial^2 A_z}{\partial x^2} + \frac{\partial^2 A_z}{\partial y^2} - \frac{1}{c^2}\frac{\partial^2 A_z}{\partial t^2} + \frac{q}{\pi\hbar}\sum_m c_m \sin\left(\frac{maq}{c}A_z(t)\right) = 0, \tag{14}$$

where the coefficients c_m can be decomposed as

$$c_m = \sum_s a_{ms}b_{ms}, \quad b_{ms} = \int_{-q_0}^{q_0}\cos(map_z)F_0(\mathbf{p})\,dp_z.$$

The numerical results showed that the expansion coefficients b_{ms} strongly decrease with increasing m at all temperatures. As shown by the classic study of one-dimensional case, the nature of the decay of a single pulse depends strongly on its velocity [25]. An increase in the relative velocity in one dimension pulses begin to interact more elastic, and some of their energy goes into vibrational modes. The general form of analytical solutions for Eq. (14) is unknown even if limit ourselves to only one term in the sum. That is why the task requires further consideration by the methods of numerical modeling.

3. Numerical simulation of the pulse dynamics

The obtained effective Eq. (14) was solved numerically using the direct difference scheme "cross" [26]. The time and coordinate steps were determined from the standard stability conditions $\Delta\tau/\Delta x < 1$. Difference scheme steps where iteratively decreased twice until the solution became unchanged in the eighth decimal place. The corresponding calculations for the one-dimensional case of the dynamics of a pulse in an array of carbon nanotubes are presented in detail in the works [7,8,27–29]. Initial pulse profile had a Gaussian form. In case when dispersion relation (2) is valid, an extremely short pulse is splitting into two, which have significantly different amplitudes. Similar behavior was observed in the study of sin-Gordon equation in nonlinear transmission lines with dispersion [25].

In this Letter we focus on the results for the pulse propagating in a system of carbon nanotubes, taking into account the impurities adsorbed on the surface of CNTs. Present study was carried out for the $(8,0)$-array of carbon nanotubes. Fig. 2 shows the pattern of electromagnetic wave propagation in an array of nanotubes with the use of both the original dispersion relation (2) and when using the model under study (5). We show the dependence of the field at different times. The dependence is typical, and it implies that the steady pulse propagation is possible in an array of carbon nanotubes. The evolution of the pulse is strongly dependent on the initial group velocity [8]. When the velocity increases, the breakaway pulse has a much smaller "area" and larger steepness of the front. Also it separates from the initial pulse later. In addition, the "faster" pulse induces a current of larger magnitude in a system of carbon nanotubes.

The study of influence of the hybridization energy V_{ak} on the pulse shape change is of particular interest, because it depends on the choice of adsorbed metal on the surface of the tube. Calculations prove that the energy of hybridization rather weakly affect (insufficiently to correct the distortions induced by the CNT) the shape of the pulse. However, the dynamics of changes made is fairly obvious: with increasing energy of hybridization V_{ak} a decrease of amplitudes of both the lagging behind and escaping waves occurs, and the escaping wave slows down.

Fig. 3 shows the distribution of the pulse field during the passage through the system of carbon nanotubes as the energy of the adsorbed atom changes. For definiteness the potential of hybridization V_{ak} is set equal to 1.43 eV.

In two dimensions the propagation of the bullets is demonstrated in Fig. 4, which shows the ratio $I/I_{\max}$ at different times. It can be seen that due to dissipation there is some blurring of the edges of the pulse, but the overall shape of the pulse is preserved. The dependence is typical, and it implies that the array of carbon nanotubes may allow for the steady propagation of pulses localized in two dimensions, which are often called in literature "light bullets" [30,31]. Our calculations showed that, although there is certain diffractive spreading of the pulse in the direction transverse to the propagation direction, the whole pulse still retains its shape. It is also important to note that there is a partial distortion of the pulse front, which is caused by diffraction.

Note that the existence of "light bullet" can be predicted proceeding from even simpler considerations. Using the property of the Lorentz invariance of Eq. (14), passing to a reference frame moving with the pulse velocity, and assuming that the pulse in the moving reference frame is $A = A(r) = A(x'^2 + y'^2)$ ((x', y') are connected to (x, y) via the Lorentz transformations), we obtain an ordinary differential equation for the vector potential:

$$\frac{d}{dr}\left(r\frac{dA}{dr}\right) + \frac{q}{\pi\hbar}\sum_m c_m \sin(maqA/c) = 0. \tag{15}$$

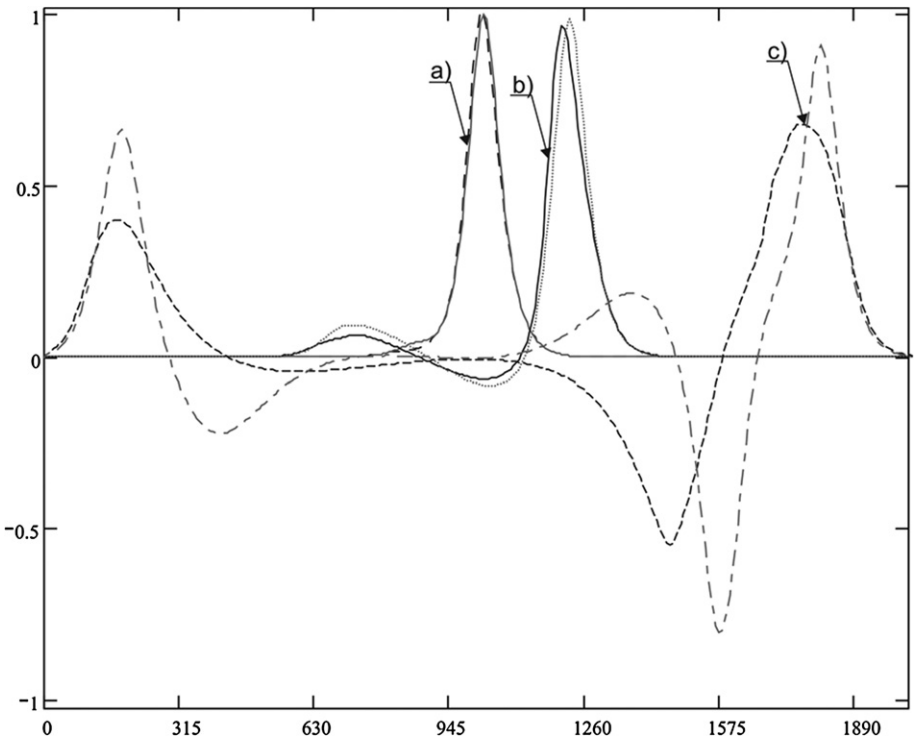

Fig. 2. Propagation profile of an electromagnetic wave in an array of nanotubes of $(8, 0)$-type for both cases, when using the original dispersion relation (2) (bright lines), and withing the frame of the discussed model (5) (dark lines). We draw the coordinate dependence of the field E at different instances of time: a) $t = 0.44 \cdot 10^{-12}$ s; b) $t = 1.48 \cdot 10^{-12}$ s; c) $t = 4.43 \cdot 10^{-12}$ s. Transverse width of the pulse is 1260 nm.

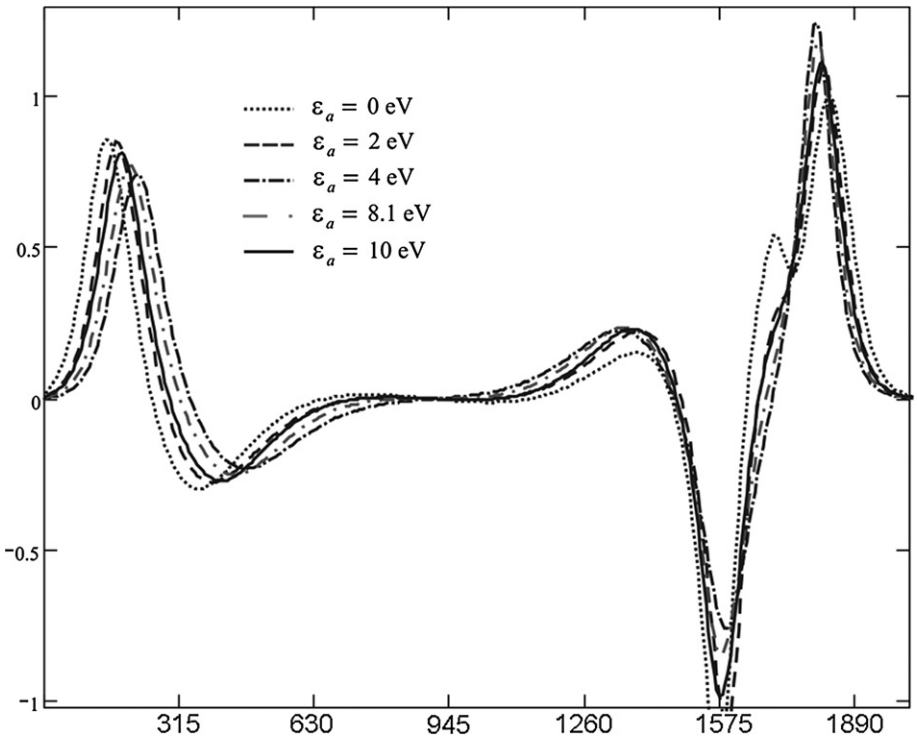

Fig. 3. Distribution of the field E of electromagnetic pulse depending on the energy of the adsorbed atom at $t = 4.43 \cdot 10^{-12}$ s for a one-dimensional problem.

Among the solutions of Eq. (15) there are solutions, which are finite at the origin and reaching a plateau at $r \to \infty$, which corresponds to a zero electric field E due to the gauge conditions.

Fig. 5 shows the intensity ratios at different energies of the adatom at time $t = 4.43 \cdot 10^{-12}$ s. At low energies the front of the main pulse becomes distorted.

It can be clearly seen that during the propagation of electromagnetic "bullet" in a simulated system of CNTs, an additional peak appears behind its front, which apparently pumps out some energy from the bullet itself. Note that this result is consistent with the results of the corresponding studies in one-dimensional case [7,29], where an additional peak was observed as well.

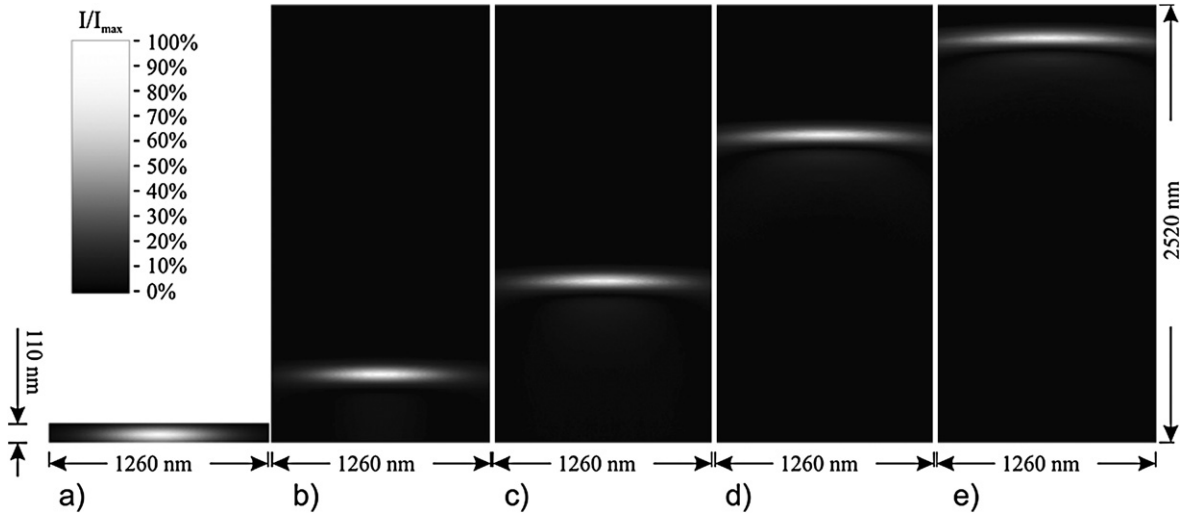

Fig. 4. Distribution of a two-dimensional pulse in the CNT, described by the dispersion relation (5). The figure represents the evolution of the ratio I/I_0. a) The initial shape of a light bullet; b) $t = 1 \cdot 10^{-13}$ s; c) $t = 1.18 \cdot 10^{-12}$ s; d) $t = 2.2 \cdot 10^{-12}$ s; e) $t = 2.88 \cdot 10^{-12}$ s.

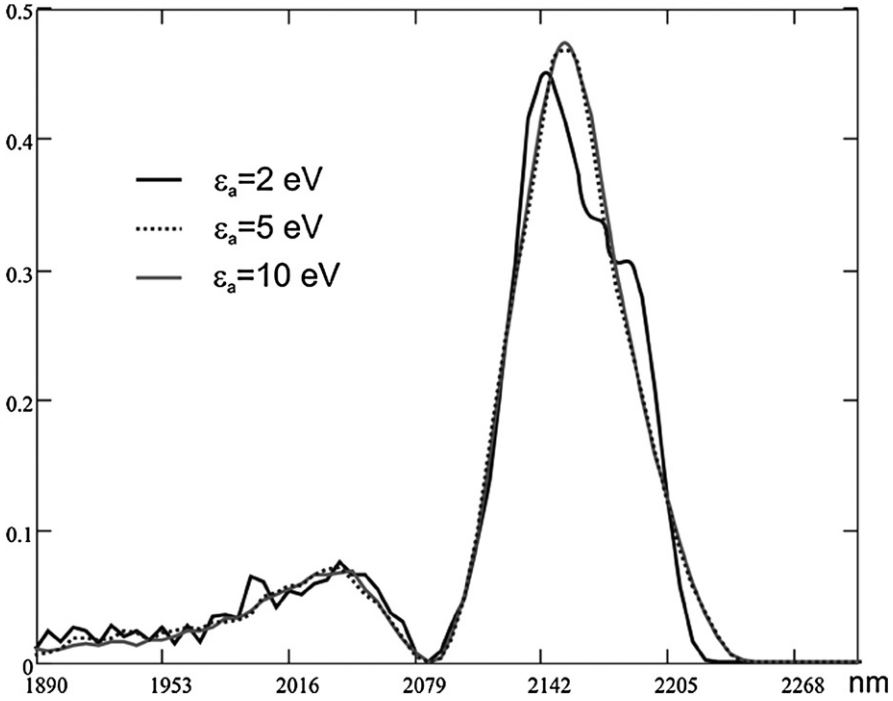

Fig. 5. Distribution of the intensity I of an electromagnetic pulse for different energies of the adsorbed atom at $t = 4.43 \cdot 10^{-12}$ s for a two-dimensional problem.

Thus, it is clear from the figure that the blurring of the pulse is relatively weak. Despite the attenuation, most of the energy is still concentrated in the center of the pulse and the light bullet is stable. The character of the intensity distribution depends on the energy of the adsorbed atom.

4. Conclusions

On the basis of the performed study the can make the following conclusions. The most important result is that unlike the one-dimensional case [32], there is a possibility of the propagation of extremely short pulses without dividing them into two parts running in opposite directions. Principally new result is the possibility of existence of light bullets in such complex structures like carbon nanotubes doped with hydrogen.

In addition, we have to mention also the following important outcomes:

(i) We proposed the model and obtained the effective equation describing the dynamics of an extremely short laser pulse in two-dimensional carbon nanotube bundles, taking into account the impurities adsorbed on the surface of carbon nanotubes;
(ii) Numerical calculations have shown that stable nonlinear waves can exist within a frame of the proposed model;
(iii) Change of the pulse shape when passing an array of CNTs strongly depends on the energy of the adatom.

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