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DYNAMICS OF ELECTROMAGNETIC PULSES WITH WIDE SPECTRA IN SEMICONDUCTOR SUPERLATTICES*

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Abstract

We considered the Maxwell equations for electromagnetic-field propagation in a solid with a one-dimensional semiconductor superlattice of quantum dots in the case where the spectral width of the electromagnetic pulse is sufficient to excite transitions between different minizones. A phenomenological equation was obtained in the form of the classical one-dimensional sine-Gordon equation with the perturbation caused by quantum transitions between the minizones. Quantum behavior of electrons was considered using the microscopic Hamiltonian, in the assumption that the pulse duration is small enough for the phonon effects to be neglected. The equation obtained was analyzed numerically, and cases where the adiabatic perturbation theory for the sine-Gordon equation can be used were found. Numerical solutions were obtained, and the domain where transitions between the minizones play a significant role in the electromagnetic-pulse dynamics was found.

Keywords: superlattice, quantum dots, minizone, sine-Gordon equation.

1. Introduction

Nowadays, electronics and related branches of science and technology are actively being developed due mainly to the miniaturization of electronic components; these developments are triggered by the discovery of new physical effects and the use of novel materials such as semiconductor quantum superlattices. The GaAs–$Al_xGa_{1-x}As$ superlattice grown by molecular-beam epitaxy was first reported in [1]. The theoretical studies of superlattices [2, 3] were performed long before they were synthesized.

The unique properties of superlattices led to intense theoretical studies and attempts to use them in nonlinear-optical devices. The main and most promising directions in this field are, in our opinion, studies of the propagation of ultrashort light pulses in superlattices (optical solitons) [4–7]. Still, processes associated with (possible) transitions of electrons between minizones in the propagation of ultrashort and extremely short pulses due to their large spectral width remained mainly outside consideration. Meanwhile, there exists a number of works with a similar range of problems related to transitions induced by optical pulses with wide spectra [8, 9], and materials used in those experiments do not belong to the class of superlattices. In short, the problem of propagation of ultimately short optical pulses characterized by a spectral width sufficient to induce transitions between the minizones is important and timely.

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2. Basic Relations and Equations

Consider a semiconductor superlattice in the geometry where the electric-field vector $\vec{E} = -\dfrac{1}{c}\dfrac{\partial \vec{A}}{\partial t}$ coincides with the superlattice axis and the electromagnetic field is linearly polarized and propagates in the direction perpendicular to the superlattice axis, i.e., along its layers.

Then the Hamiltonian of the system of electrons can be written as follows:

$$\begin{aligned} H &= H_0 + H_t, \\ H_0 &= \sum_{ps} \varepsilon_s \left(p - \frac{e}{c}A(t)\right) a^{\dagger}_{ps} a_{ps}, \\ H_t &= -\frac{e}{c}\frac{\partial A}{\partial t} \sum_{pss'} M_{ss'}(p) a^{\dagger}_{ps} a_{ps'} + \text{c.c.}, \end{aligned} \tag{1}$$

where $a^{\dagger}_{ps}$ and a_{ps} are the creation and annihilation operators of electrons with momentum p in an sth minizone, $A(t)$ is the vector potential of the electromagnetic field directed along the superlattice axis, $\varepsilon_s(p)$ is the electron dispersion law in the sth minizone with momentum p directed along the superlattice axis, and $M_{ss'}(p)$ is the matrix element of the transition with momentum p from the sth minizone to the s'th minizone. Note that the expression for H_0 does not include the summand depending on momenta of electrons in the directions perpendicular to the superlattice axis $p^2_{\perp}/2\,m_{\text{eff}}$, where m_{eff} is the corresponding effective mass. One can see that this summand commutes with the system Hamiltonian given by (1) and thus does not influence the further calculations.

The electron dispersion law in the sth minizone with momentum p is chosen in the form

$$\varepsilon_s(p) = \varepsilon_{0s} - d_s \cos(ap),$$

where d_s is the minizone width and a is the superlattice constant.

Since we consider ultrashort optical pulses, we can neglect the summands describing the interaction of the electron and photon subsystems in the Hamiltonian (1). The expressions for $M_{ss'}(p)$ are given in [10] where it is also shown there that indirect transitions are forbidden in the case under consideration. We will number the minizones starting with the minizone with the smallest energy. Assuming that in the spectral domain the ultrashort optical pulse is restricted by the values of $\max\Big(\varepsilon_3(p) - \varepsilon_2(p)\Big)$ from below and $\min\Big(\varepsilon_{N+1}(p) - \varepsilon_1(p)\Big)$ from above, further we will consider only the transition scheme corresponding to the V scheme in the terminology accepted in optics. In this scheme, only transitions from the lowest minizone to all the other minizones are allowed; all the others are forbidden. Note that in this case the restriction is valued not only for the matrix elements $M_{ss'}(p)$ but for the spectral width of the pulse and, consequently, for its duration.

We write the expression for the current in the traditional form [11]:

$$j = e\sum_{ps} \nu_s \left(p - \frac{e}{c}A(t)\right) \langle a^{\dagger}_{ps} a_p s\rangle, \tag{2}$$

where $\nu_s(p) = \partial\varepsilon_s(p)/\partial p$ and the brackets denote averaging in view of the nonequilibrium density matrix $\rho(t)$

$$\langle B\rangle = \text{Sp}\Big(B(0)\rho(t)\Big).$$

In the considered geometry, the electromagnetic field is described classically based on the Maxwell equations. Thus, in the case of interest, taking into account the dielectric and magnetic properties of the system considered, the Maxwell equations can be written as follows [12]:

$$\frac{\partial^2 A}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} + \frac{4\pi}{c} j = 0, \tag{3}$$

where x is the direction of the ultrashort-pulse propagation and instead of the vectors their projections on the superlattice axes are written.

In view of the equation for the density matrix $\rho(t)$, the equations for mean values of the operators $\langle a^\dagger_{ps} a_p s' \rangle$ can be presented as the system of ordinary differential equations in the matrix form

$$\frac{\partial L}{\partial t} = i(EL - LE), \tag{4}$$

where matrices L and E are

$$L = \begin{vmatrix} \langle a^\dagger_{p1} a_{p1} \rangle & \langle a^\dagger_{p1} a_{p2} \rangle & \langle a^\dagger_{p1} a_{p3} \rangle & \dots \\ \langle a^\dagger_{p2} a_{p1} \rangle & \langle a^\dagger_{p2} a_{p2} \rangle & \langle a^\dagger_{p2} a_{p3} \rangle & \dots \\ \langle a^\dagger_{p3} a_{p1} \rangle & \langle a^\dagger_{p3} a_{p2} \rangle & \langle a^\dagger_{p3} a_{p3} \rangle & \dots \\ \dots & \dots & \dots & \dots \end{vmatrix}, \qquad E = \begin{vmatrix} e_{p1} & M12V & M_{13}V & M_{14}V & \dots \\ M_{12}V & e_{p2} & 0 & 0 & \dots \\ M_{13}V & 0 & e_{p3} & 0 & \dots \\ M_{14}V & 0 & 0 & e_{p4} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{vmatrix},$$

with

$$e_{pi} = \varepsilon_i \left(p - \frac{e}{c} A(t) \right), \qquad V = -\frac{e}{c}\frac{\partial A}{\partial t}, \qquad M_{1i} = M_{1i}(p).$$

In this case, it is evident that

$$L(t) = S(t) L(0) S^\dagger(t), \qquad \frac{\partial S(t)}{\partial t} = iES(t).$$

Representing $E = E_0 + E_1$, where $E_0 = \mathrm{diag}|, (e_{p1}, e_{p2}, \dots)$, we obtain that

$$S = \exp\left(i \int_{-\infty}^{t} E_0(t') dt' \right) S_1, \qquad \frac{\partial S_1}{\partial t} = iQS_1, \tag{5}$$

where the matrix Q is defined as

$$Q = \begin{vmatrix} 0 & Q12 & Q_{13} & Q_{14} & \dots \\ Q^*_{13} & 0 & 0 & 0 & \dots \\ Q^*_{14} & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 \end{vmatrix}, \qquad Q_1 = \exp\left(-i \int_{-\infty}^{t} (e_{p1} - e_{pj}) dt' \right) M_{1j} V,$$

and the star denotes the complex conjugate. To solve the equation for the matrix S_1, we use the quasi-classical approximation [13, 14] developed just for the case of ultrashort pulses propagating in resonant multilevel media, i.e., instead of the exact solution of Eq. (5) in the form

$$S_1(t) = T \exp\left[i \int_{-\infty}^{t} Q(t')\, dt' \right], \tag{6}$$

we write an approximate solution in the form

$$S_1(t) = \lim_{t\to t_0, \|Q\|\to\infty} \exp\left[i \int_{t_0}^{t} Q(t')\, dt' \right], \tag{7}$$

where $\|Q\|$ is the norm of the matrix operator Q. The justification of this approximation is that, when calculating the solution of Eq. (5), e.g., by the Magnus expansion method, one encounters expressions of the form $\int_0^t \int_0^{t_1} dt_2 dt_1 \,[Q(t_2), Q(t_1)]$ with commutators in some sense small (due to the very small pulse duration) and can be neglected. A detailed analysis with the mathematically correct conditions for the application of such approximation is given in [14]. Following the formalism developed in [13,14] and taking into account that the matrix $R = 2\int_{-\infty}^{t} Q(t')\, dt'$ satisfies the relation

$$R^3 = h^2 R,$$

where

$$\begin{aligned} h^2 &= |R_{12}|^2 + |R_{13}|^2 + |R_{14}|^2 + \cdots, \\ R_{1j} &= 2\int_{-\infty}^{t} \exp\left[-i \int_{-\infty}^{t'} (e_{p1} - e_{pj})\, dt'' \right] M_{1j} V(t')\, dt', \end{aligned}$$

it is easy to obtain that

$$S(t) = I - 2\,\frac{R^2}{h^2} \sin^2\frac{h}{4} + i\,\frac{R}{h} \sin\frac{h}{2},$$

with I a unit matrix.

The expressions for mean values $\langle a^\dagger_{ps} a_{ps}\rangle = n_{ps}$, in view of the fact that only the means $\langle a^\dagger_{ps} a_{ps'}\rangle$ with $s = s'$ were different from zero at the initial moment of time, read

$$\begin{aligned} n_{p1} &= n^0_{p1} \cos^2\frac{h}{2} + \sum_j \left[\frac{R_{1j}}{h}\right]^2 n^0_{pj} \sin^2\frac{h}{2}, \\ n_{pj} &= n^0_{pj} + \left[\frac{R_{1j}}{h}\right]^2 \left[n^0_{p1} \sin^2\frac{h}{2} - 4 n^0_{pj} \sin^2\frac{h}{4} + 4\sum_{k\neq 1} n^0_{pk} \left[\frac{R_{1j}}{h}\right]^2 \sin^4\frac{h}{4} \right], \end{aligned} \tag{8}$$

where n^0_{p1} and n^0_{pj} are the equilibrium mean values of the occupation numbers with moment p in the first and jth minizones. Note that Eq. (3), taking into account (2) and (8), converts into a phenomenological equation for the vector potential A, which completely describes the model we proposed.

3. Some Approximations and Numerical Analysis of the Phenomenological Equation

The phenomenological equation obtained can be simplified, e.g., for the case of low temperatures, assuming that electrons are in the first minizone only, and the upper minizones are not occupied. If the dispersion law $\varepsilon_s(p) = \varepsilon_{0s} - d_s \cos(ap)$, and having in mind the symmetry of the problem, we write the phenomenological equation as

$$\frac{\partial^2 A}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} - \frac{4\pi e d_1 a}{c} \sin\left(\frac{eA}{c}\right) \sum_p n_{p1}^0 \cos(ap) \left[\cos^2\frac{h}{2} + \sum_j \frac{d_s R_{1j}^2}{d_1 h^2} \sin^2\frac{h}{2}\right] = 0. \qquad (9)$$

We obtain that, in the absence of transitions, Eq. (9) exactly coincides with the equation for the dynamics

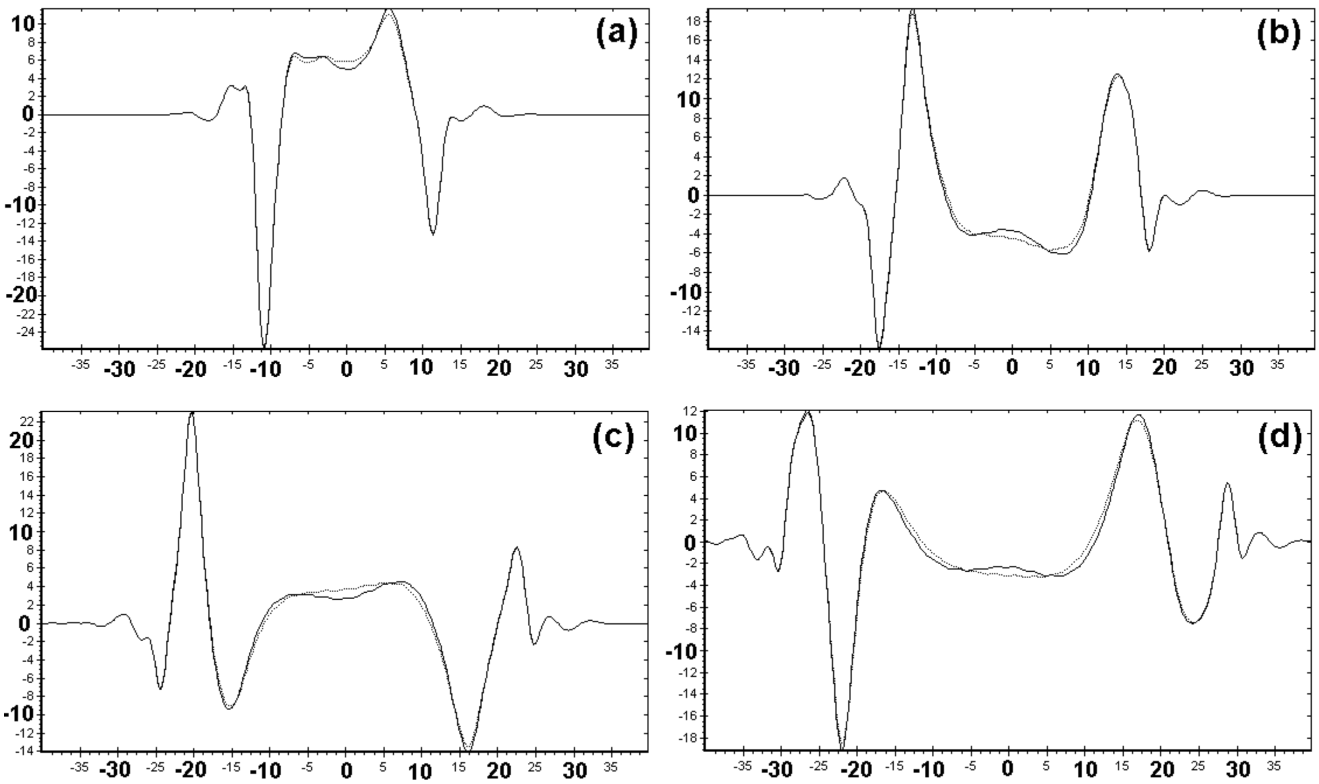

Fig. 1. Dynamics of the electromagnetic field in a superlattice in the consideration of the electron transitions between minizones. The matrix elements of transitions are taken to be zero (dashed curves) and calculated from [10] (solid curves). The electric field in relative units $[eEa\tau/\hbar]$ is shown at the axis y and the coordinate in relative units $[\chi/a]$ is shown at the axis x; $t = \tau$ (a), $t = 1.5\,\tau$ (b), $t = 2\,\tau$ (c), and $t = 2.5\,\tau$ (d).

of the electromagnetic field (in a semiconductor superlattice) in the one-minizone approximation derived in [15]; it has the form of the sine-Gordon equation, for which analytical methods are well known [16,17]. A far more nontrivial fact is that, if all minizones are of the same width ($d_1 = d_s$), the expression obtained also has the form of the sine-Gordon equation. This enables one to use the perturbation theory [18,19] developed for the sine-Gordon equation in our case, as well, using the value $(1 - d_s/d_1)$ as a small parameter. Note that this small parameter is in no way related to the optical pulse parameters and is determined only by the geometry of the superlattice layers. This fact has a rather simple physical interpretation. Within the framework of our model, the coherent transitions are considered and relaxation processes are neglected. Herewith, electrons transit coherently from one minizone to the other and back with the phase preserved due to the equality of the minizones' widths, and the pulse behaves similarly to the pulse in a superlattice within the framework of one-minizone approximation.

We solved the equation numerically using the cross-type direct finite-difference scheme [20]. Time and coordinate steps were determined from the standard stability conditions. The finite-difference scheme steps were decreased consecutively by one-half until the solution did not change in the eighth digit.

As an example, we consider the modeling results for a structure with the lattice constant $a = 8{\cdot}10^{-6}$ cm and the static dielectric constant $\varepsilon = 31.25$ at a temperature of 40 K for two possible transitions with energy levels $\varepsilon_{01} = 2{\cdot}10^{-14}$ erg, $\varepsilon_{02} = 8{\cdot}10^{-14}$ erg, and $\varepsilon_{03} = 32{\cdot}10^{-14}$ erg. The other parameters are as follows: the potential well width is $4{\cdot}10^{-6}$ cm, the potential well depth $U_0 = 80{\cdot}10^{-14}$ erg, the widths of the minizones of superlattice conductance $d_1 = 1{\cdot}10^{-14}$ erg, $d_2 = 4{\cdot}10^{-14}$ erg, and $d_3 = 8{\cdot}10^{-14}$ erg. Herewith, the matrix elements of transitions, calculated according to [10], were estimated to be $M_{12} = 0.0070114$ and $M_{13} = 0.0385405$. The electromagnetic-field pulse was given in the form

$$E(t) = E_0 \sin(wt) \exp\Big(- \alpha^2 (x - ct/\varepsilon)^2 \Big). \tag{10}$$

The field amplitude $E_0 = 1.5{\cdot}10^5$ V/m and the frequency $\omega = 3{\cdot}10^{14}$ s^{-1}; the constant α determining the duration was chosen to be equal to 0.4, whereas the pulse contained only three oscillations. The time scale τ presented in the figures is determined by the ratio $\tau = 1/\omega$.

The pulse evolution is presented in Fig. 1.

As is expected for systems described by equations close to the sine-Gordon equation, the initial perturbation decomposes into two localized states, which are close to the breathers of the sine-Gordon equation. These states, similar to the breathers and consisting of a small number of oscillations, propagate subsequently without changing their form, since they are close to the soliton solutions of the sine-Gordon equation. As seen in the plots, consideration of transitions between the minizones proves to have the strongest effect on the decomposition of the initial state; the main distinction between the cases of the presence and absence of electron transitions between the minizones is focused in the domain of the initial localization of the optical pulse.

Note that similar dependences were also obtained at other values of the superlattice parameters. Thus, Fig. 2 presents the results of modeling for a structure different from that described above by the electron concentration in the first minizone; the concentration increases 10 times.

It is easy to see that the solutions (analogs of breathers) are more pronounced in Fig. 2, which is due to the increased nonlinearity owing to the increase in the electron concentration in the first minizone. The decomposition of the initial state of the electromagnetic field and the formation of stable solutions analogous to the breathers have, in our opinion, a simple physical interpretation. Initially, the electromagnetic-field pulse has a wide spectrum, which also includes frequencies corresponding to the frequencies of transitions between the minizones. Electrons start to perform transitions between the minizones, and at this point the electromagnetic field is absorbed at frequencies corresponding to the frequencies of the transitions, and the pulse propagates further without corresponding harmonics in its spectral decomposition. As a consequence of reverse transitions in the domain where the pulse initially was, the electromagnetic field is generated again and starts to interfere with the tail of the solution of a breather analog already propagated further, which is what yields the pattern observed. Note that, since the absorption of the electromagnetic field and the further reappearance of the field due to reverse transitions occur in a rather narrow spectral domain, its effect on the pulse shape in the time domain is correspondingly small. Thus, in the domain where the electromagnetic-field pulse was initially

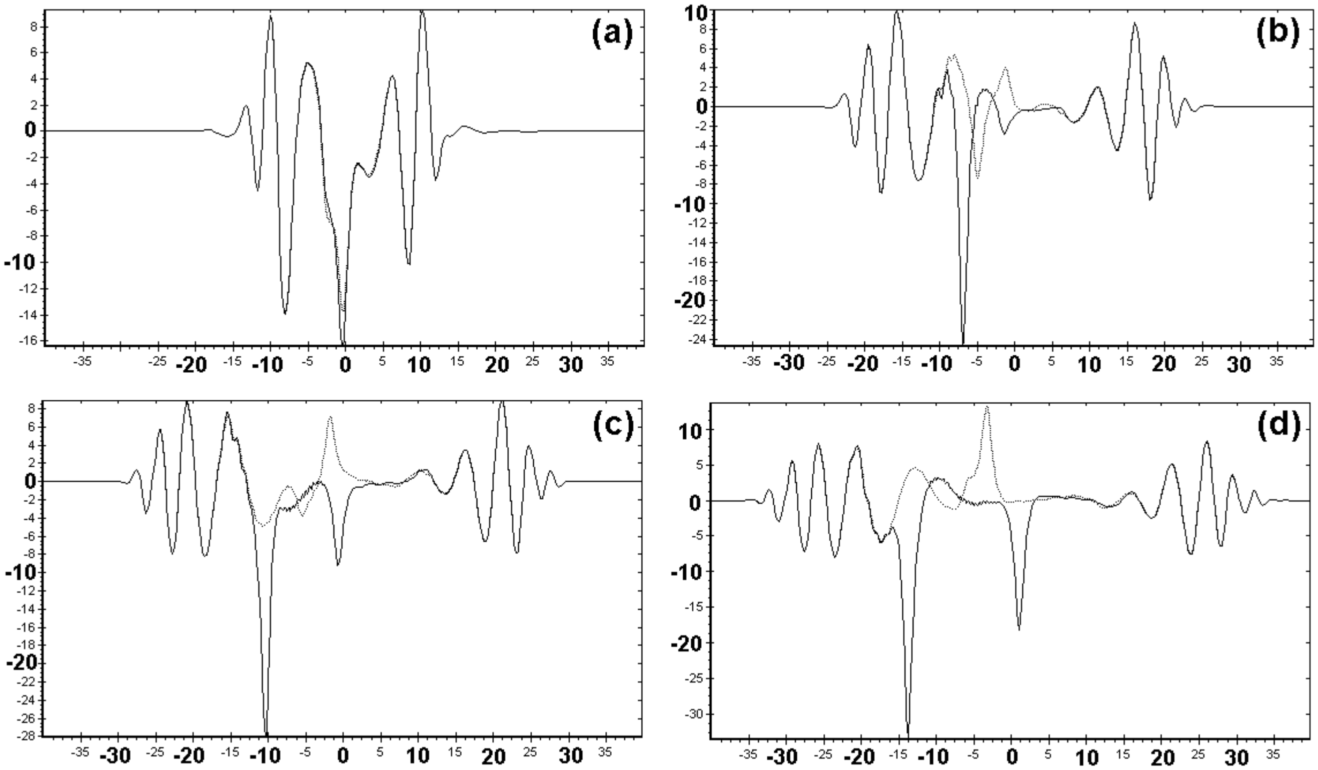

Fig. 2. Dynamics of the electromagnetic field in a superlattice in the consideration of electron transitions between minizones. The matrix elements of transitions are taken to be zero (dashed curves) and calculated from [10] (solid curves). The electric field in relative units $[eEa\tau/\hbar]$ is shown at the axis y and the coordinate in relative units $[\chi/a]$ is shown at the axis x; $t = \tau$ (a), $t = 1.5\,\tau$ (b), $t = 2\,\tau$ (c), and $t = 2.5\,\tau$ (d). The electron concentration increases 10 times in comparison with presented in Fig. 1.

localized, an analog of the spectral filtration of the electromagnetic-field pulse occurs owing to electron transitions between the minizones. Then the pulse propagates without the effect of the processes caused by the electron transitions between the minizones. As proof of the model proposed, we present the time dependence of the value

$$F = \sum_p \cos(ap) \left[\cos^2\frac{h}{2} + \sum_j \frac{d_s R_{1j}^2}{d_1 h^2}\sin^2\frac{h}{2}\right],$$

which describes the electron transitions between the minizones caused by the oscillating electromagnetic field (see Fig. 3).

Note that, if we take the matrix elements of the transitions to be equal to zero, the calculated value F for the chosen parameters should be 0.19628. It is easy to see that this value describing the electron transitions between the minizones differs significantly from the case of the absence of transitions in the domain where the pulse was initially concentrated and in the domains for the solutions analogous to the breathers. The latter circumstance is related just to the emergence of the electromagnetic field at corresponding frequencies, which, in turn, causes new transitions.

The consideration of possible electron transitions between the minizones in the case of an optical pulse

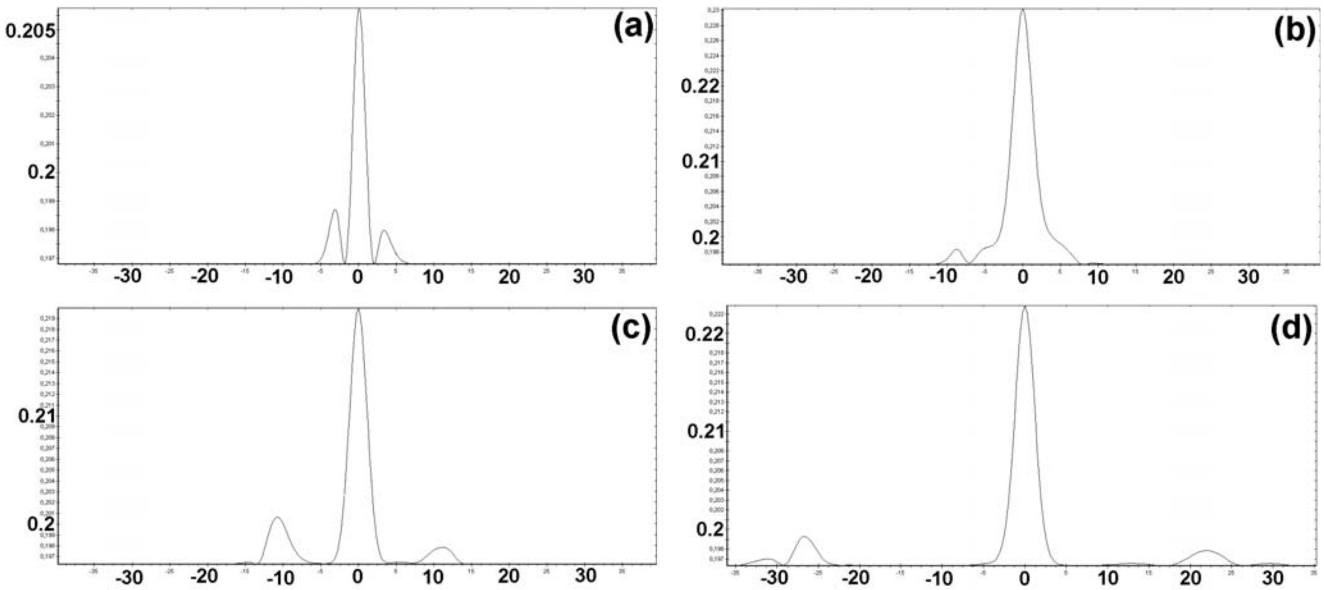

Fig. 3. Dynamics of the value F (the axis y) in the consideration of electron transitions between minizones. The coordinate in relative units $[\chi/a]$ is shown at the axis x; $t = 0.2\,\tau$ (a), $t = 0.7\,\tau$ (b), $t = 1.1\,\tau$ (c), and $t = 2.8\,\tau$ (d). The structure parameters are the same as in Fig. 1.

with wide spectrum is essential at the initial stage of the pulse evolution. Subsequently, the initial pulse decomposes into localized states (analogs of breathers), and the effects associated with the consideration of electron transitions play a significant role already after the localized state is passed. This, in turn, leads to an increase in the pulse duration.

4. Conclusions

In conclusion, we summarize the main results obtained in this study.

- A phenomenological equation describing the electromagnetic field dynamics was derived for the case where it is important to take into account the electron transitions between minizones in a superlattice caused by the oscillating field of the pulse.

- It was shown that, in the case where the minizones were of approximately equal widths, the problem could be considered based on the perturbation theory for the sine-Gordon equation, and the role of the smallness parameter was played by the ratio of the difference of the minizones' widths to the width of the first minizone.

- It was shown that the ultrashort optical pulse decomposed into solutions analogous to the breathers; the effects associated with the electron transitions were significant only in the domain of the initial-pulse localization.

- In the domain where the electromagnetic pulse was initially localized, as a consequence of electron transitions between minizones, an analog of spectral filtration of the electromagnetic field pulse arised. Further on, the pulse propagated as if experiencing no impact on the part of the processes caused by the electron transitions between the minizones.

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