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PECULIARITIES OF SOLITON EXCITATIONS IN THE In_4Se_3 CRYSTAL

We present new investigations of the spatially localized excitations of soliton type in the framework of the nonlinear Schrodinger equation. It is shown that the fourth - order effects are crucial for the formation of solitary waves in the layered In_4Se_3 crystal. The balance between the higher order dispersive terms and nonlinearity, induced by lattice deformation, may lead to the different spatial localized excitations. They can be stable or unstable depending on the parameters of the dispersion law and the wave vector region. It is found that one- soliton and multisoliton solutions can be realized in the In_4Se_3 crystal. The parameters of soliton excitations (energy, amplitude, velocity) have been determined. The time evolution of soliton was investigated too.

Keywords: Dispersion law with low-energy non-parabolicity; Fourth-order dispersive nonlinear Schrodinger equation; Soliton excitation

Introduction

Nowadays there are different equations types for the investigation of the soliton excitations in the nonlinear systems. As it is known the Davydov' soliton theory was more widely developed for the one-dimensional (quasi-dimensional) structures [1, 2] where electron-phonon interaction is essential. Solitons as solitary spatial localized excitations were successively used for the explanations of many physical and chemical phenomena, in particular, the phenomena related to the energy transfer in the biological systems. Bisoliton model of the high-temperature superconductivity and the existence of the nonlinear waves, connected with the electron-phonon interaction in the layered crystal [3], were also based on the simple models of the one-dimensional molecular crystal. However, the autolocalized state of soliton type can be formed in the anisotropic two-dimensional structures at the definite physical parameters too [4].

Traditionally, solitons in the condensed state physics are studied on the base of the nonlinear Schrodinger equation with the spatial two-order derivatives. But there are the real systems where the integral dynamical equations don't give the adequate description of the physical characteristics, for instance, prediction of the ultrashort optical pulses in solid-state lasers, optical solitons in Kerr'law media, solitons in plasma, optical solitons in the fibers [5-7]. For their explanations, it is necessary to modify the nonlinear Schrodinger equation by the means of the inclusion of higher-order dispersion terms.

It is of considerable interest to study the nonlinear mechanics of the solitary waves in the discrete atomic systems where the frequency contains the higher orders of the wave vector components that results in the occurrence of the spatial fourth-order derivatives in the nonlinear Schrodinger equation. The peculiarities of dynamical solitons in such nonlinear systems were considered in the papers by Kosevich [8, 9]. The magnetic solitons within differential equation with fourth –order term were also investigated in [10].

It is shown that the higher dispersive effects may cause significant qualitative changes in the dynamics of nonlinear structures. From this point of view, it is of interest to investigate the soliton excitations in the layered In_4Se_3 crystal, for which the nonlinear Schrodinger equation with the fourth-order dispersion takes place owing to the nonstandard dispersion law for charge carriers [11-15]. Moreover, explanation of the inherent in this crystal dynamical disordering is related with the electron-phonon interaction and possibility of the nonlinear wave realization in the normal to layers direction [16].

As it is known the In_4Se_3 semiconductor is a unique three-dimensional periodic system with the interesting physical properties [17-19]. The interaction between an electron and the longitudinal acoustic phonon leads to the localized electron state in the form of condenson in this crystal [11, 20]. As opposed to polar or ionic crystals, the condenson states being the analogs excitations of polarons arise, according to the theory by Deigen and Pekar, in homopolar dielectrics [21]. In other three-dimensional crystals whose charge carriers are described by ordinary parabolic dispersion law, the condenson state cannot arise. The condition for the condenson states is fulfilled in 3D- In_4Se_3 crystal due to its peculiar dispersion law for charge carries, which contains the second and fourth order components of the wave vectors, and to the peak-like density of electron states [11]. In the first time, the concept of condenson states in the three-dimensional In_4Se_3 crystal was used for the explanation of the high thermoelectric performance [22,23], which appeared to be larger than 1.4 at 705 K [18]. Experimental investigations of the charge and thermic transport suggest the existence of the condenson states in the In_4Se_3 layered crystal [22, 23].

It is noted that the dispersion law with low-energy non-parabolicity is also used for an explanation of some peculiarities of the kinetic [24] and optical [15,25] properties in the In_4Se_3 crystal. In the [26] the scattering of the waves by the planar defects in the semiconducting crystals utilized the model dispersion law has been studied. Due to the space dispersion, a new effect of the wave total reflection from the interfaces has been founded. It allows considering the In_4Se_3 crystal as a promising material for chalcogenide waveguides.

In the present study, we study the possibilities of the appearance of the different spatial localized excitations of soliton type and analyze their spatial and time evolutions in the In_4Se_3 crystal.

Hamiltonian system in the continual approach and the nonlinear Schrodinger equation with fourth-order dispersion

As it is followed from long-time our investigations [11-15], the dispersion law for the charge carriers in the In_4Se_3 crystal in the vicinity of the band gap is characterized by the low-energy non-parabolicity connected with opposite sign of the coefficients at the second and fourth order components of the wave vectors:

$$E\left(\vec{k}\right) = -\alpha_1 k_x^2 - \alpha_2 k_y^2 - \alpha_3 k_z^2 + \beta_1 k_x^4 + \beta_2 k_y^4 + \beta_3 k_z^4 \qquad (1)$$

where $\beta_i >> \alpha_i \;\; i = 1,2,3$. As follows from (1), for the smallest wave vector $\vec{k}$ (to the $k_0 = \pm\left(\alpha_i / 6\beta_i\right)^{1/2}$ point) the region of the negative curvature is observed in the vicinity of the Brillouin zone center, and the parabolicity is restored with an increase of $\vec{k}$. The absolute extrema are displaced in the $k_{0m} = \pm\left(\alpha_i / 2\beta_i\right)^{1/2}$ points and depth of the band minimum is determined by the expression $E_m = -\alpha_i^2 / 4\beta_i$. Owing to such complicated energy, dependence on the wave vectors the different energy ranges can be utilized for the investigation of the soliton excitations in the In_4Se_3 crystal.

Let us write the Hamiltonian for the system taking into account the interaction energy between the electron and local deformation. It is assumed that the local deformational interaction is strong and the particle movement is accompanied by the displacement atoms from the equilibrium position. Then local displacement is the potential well which holds the electron.

Following to Davydov‘ theory [1, 2] in the continual approach Hamiltonian has the form:

$$H = H_{el} + H_{el-def} + H_{pot} + H_{kin} \qquad (2)$$

where

$$H_{el} = \int \Psi^*(\vec{r},t)\left(\alpha_i \nabla^2 + \beta_i \nabla^4\right)\Psi(\vec{r},t)\, d^3\vec{r}\,,$$

$$H_{el-def} = -\int \sum_{ij} b_{ij}\varepsilon_{ij} |\Psi|^2 d^3\vec{r}\,,$$

$$H_{pot} = \frac{1}{2}\sum_{ijkl}\lambda_{ijkl}\varepsilon_{ij}\varepsilon_{kl}\,, \quad H_{kin} = \frac{1}{2}M\sum_i\left(\frac{\partial u_i}{\partial t}\right)^2.$$

Here b_{ij} are components of the deformation potential tensor, λ_{ijkl} are the elastic moduli, M is a mass atom, u_i is the displacement of i-atom, $\frac{\partial u_i}{\partial t}$ is the velocity of i-atom, $\varepsilon_{ij} = -a_i\frac{\partial u_i}{\partial x_j}$, $\varepsilon_{kl} = -a\frac{\partial u_k}{\partial x_l}$ are deformation tensor components. Utilizing (2), a functional $E = \langle\Psi|H|\Psi\rangle$ has the form:

$$E\{\Psi,\rho(x,t)\} = \int\left[-\alpha_i(\nabla\Psi)^2 + \beta_i\left(\nabla^2\Psi\right)^2 - \sum_{ij} b_{ij}\varepsilon_{ij}|\Psi|^2 + \frac{1}{2}\sum_{ij}\lambda_{ijkl}\varepsilon_{ij}\varepsilon_{kl} + \frac{1}{2}M\sum_i\left(\frac{\partial u_i}{\partial t}\right)^2\right]d^3\vec{r} \qquad (3)$$

Variating (3) on Ψ-function and then on u_i-displacement we obtain two equations, which determine the electron localized states in the In_4Se_3 crystal:

$$\left[i\hbar\frac{\partial}{\partial t} - \alpha_i\nabla_i^{\,2} - \beta_i\nabla_i^{\,4} + \sum_i b_i\varepsilon_i\right]\Psi = 0\,,$$

$$\left(\frac{\partial^2 u}{\partial t^2} - \sum_k \lambda_{ik}\frac{a^2}{M}\frac{\partial^2 u_k}{\partial x_i \partial x_k}\right) + \frac{b_i a}{M}\frac{\partial}{\partial x}|\Psi|^2 = 0\,. \qquad (4)$$

In the new coordinate system $\xi = (x - vt)/a$, $\eta = y/b$, $\varsigma = z/c$ (a, b, c are the lattice parameters of the In_4Se_3 crystal, v is the velocity of the excitation spreading along the definite direction, for instance, x-direction) the second equation of (4) will be described by the expressions:

$$\left(\frac{v^2}{a^2}\frac{\partial^2}{\partial\xi^2} - \frac{V_{01}^2}{a^2}\frac{\partial^2}{\partial\xi^2}\right)\varepsilon_1 + \frac{b_1}{Ma}\frac{\partial^2}{\partial\xi^2}|\Psi|^2 = 0\,,$$

$$-\frac{V_{02}^2}{b^2}\frac{\partial^2}{\partial\eta^2}\varepsilon_2+\frac{b_2}{Mb}\frac{\partial^2}{\partial\eta^2}\left|\Psi\right|^2=0,$$

$$-\frac{V_{03}^2}{c^2}\frac{\partial^2}{\partial\varsigma^2}\varepsilon_3+\frac{b_3}{Mc}\frac{\partial^2}{\partial\varsigma^2}\left|\Psi\right|^2=0\ . \quad (5)$$

Here $V_{01}^2=\frac{\lambda_{11}a^2}{M}$, $V_{02}^2=\frac{\lambda_{22}b^2}{M}$, $V_{03}^2=\frac{\lambda_{33}c^2}{M}$ are the sound longitudinal velocities in the general directions. From (5) it is easy to determine $\varepsilon_1, \varepsilon_2$ and ε_3, which are equal to

$$\varepsilon_1=\frac{b_1}{a^2\lambda_{11}\left(1-\frac{v^2}{V_{01}^2}\right)}\left|\Psi\right|^2,\ \ \varepsilon_2=\frac{b_2}{b^2\lambda_{22}}\left|\Psi\right|^2,\ \varepsilon_3=\frac{b_3}{c^2\lambda_{33}}\left|\Psi\right|^2.$$

Substituting these expressions into the first equation of (4), we obtain the nonlinear Schrodinger equation with the spatial fourth-order derivatives:

$$\left[i\hbar\frac{\partial}{\partial t}-\alpha_i\nabla_i^{\,2}-\beta_i\nabla_i^{\,4}+G\left|\Psi\right|^2\right]\Psi=0 \quad (6)$$

where $G\left|\Psi\right|^2=\sum_i b_i\varepsilon_i$ and $G=\sum_i\frac{b_i^2}{a_i^3\lambda_{ii}}$ (for $v<<V_{01}$) is the media nonlinearity parameter connected with the electron-phonon interaction. According to our valuation on the basis of known parameters of the deformation potential $b_i=10$eV and the generalized elastic moduli $\lambda=1.5\cdot10^{29}$ eV/m^3 [11], for the In_4Se_3 crystal, the nonlinearity parameter is equal to the $G=1$eV.

Numerical simulation of the soliton excitations in the In_4Se_3 crystal

For the numerical investigations of the nonlinear equation with the fourth-order dispersion, the different solitary wave ansatz has been proposed [5, 27]. In our investigation we shall adopt the ansatz solution in the form:

$$\Psi\left(x,t\right)=\Phi(x,t)e^{i(kx-\omega t)} \quad (7)$$

where

$$\Phi=\frac{A}{ch^2B\left(x-vt\right)}. \quad (8)$$

Let us illustrate further (similar to [27]) that considered functions can be described the soliton solutions of nonlinear Schrodinger equation in the spatial derivatives (6). The successive substation (7) and (8) in equation (6) leads to a system of the three equations which allows determining the parameters of soliton excitations:

$$\left\{\left(E+\alpha k^2-\beta k^4\right)+4B^2\left(-\alpha+6\beta k^2\right)-16\beta B^4\right\}\frac{A}{ch^2B(x-vt)}=0,$$

$$\left\{-6\left(-\alpha+6\beta k^2\right)+120\beta B^2\right\}\frac{AB^2}{ch^4B(x-vt)}=0, \qquad (9)$$

$$\left(-120\beta B^4+GA^2\right)\frac{A}{ch^6B(x-vt)}=0.$$

As follows from (9) soliton energy is defined by the expression:

$$E=-\alpha k^2+\beta k^4-4B^2(-\alpha+6\beta k^2-4\beta B^2) \qquad (10)$$

and amplitude, frequency is described by the relationships accordingly:

$$A=\sqrt{\frac{120\beta B^4}{G}},\quad B=\sqrt{\frac{-\alpha+6\beta k^2}{20\beta}}\ . \qquad (11)$$

The soliton velocity is determined as

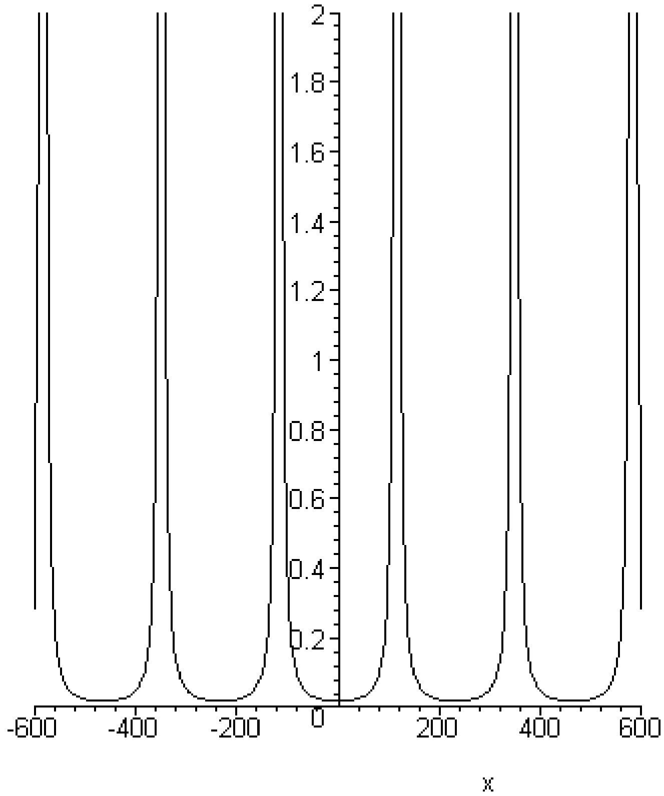
$$v=-2\alpha k+4\beta k^3-16B^2\beta k. \qquad (12)$$

Using (11) and (12), the dependencies $\psi(x,t)=\dfrac{A}{\mathrm{ch}^2 B\left(x-vt\right)}e^{i(kx-wt)}$ for the different parameters of the dispersion law (1) at the different wave vector and time values are presented in Fig.1-5. The parameters of dispersion law (1) are taken from papers [12, 13,15].

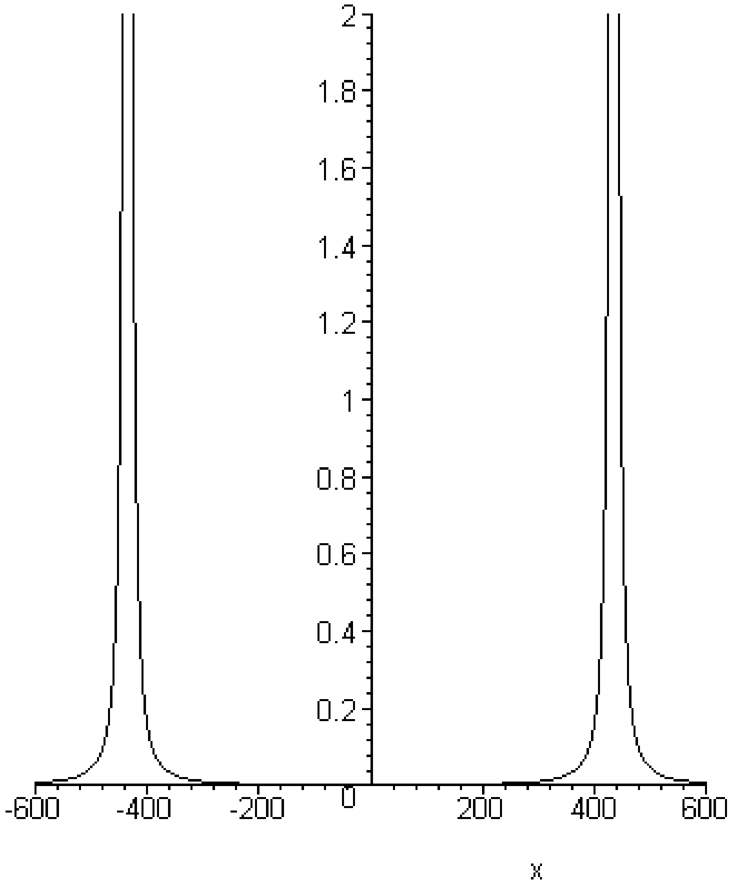
As it is shown in Fig.1 the soliton solutions in the considered energy range with the negative curvature are absent. The period of this function depends on the dispersion law parameters (1).

We also obtained the functional dependence $\psi(x)$ for the energy range, where terms at the different order of the wave vector components in the dispersion law (1) are nearly equal (Fig.2).

The damping oscillatory shape with the separated peaks in the distance is the important feature of the considered function dependencies, similar to ones found by Kawahara [28]. As it is marked in [28] such solution containing more than one peak can be considered as bound states of the soliton, and the soliton was called “multisoliton”. At the energy corresponding to the displaced extremum minima in the energy spectrum of the In_4Se_3 crystal, the solution of the (6) is one soliton (Fig.3). The time dynamics of solitons is presented in Fig.4 (a-d). As follows from these figures, the both the soliton movement and the change of its amplitude take place. Fig. 5 demonstrates the dependence of the function $\psi(k,x)$ on the wave vector ($k=0\div 0.25$) for the dispersion law parameters $\alpha_2=13$ eV, $\beta_2=888$ eV.

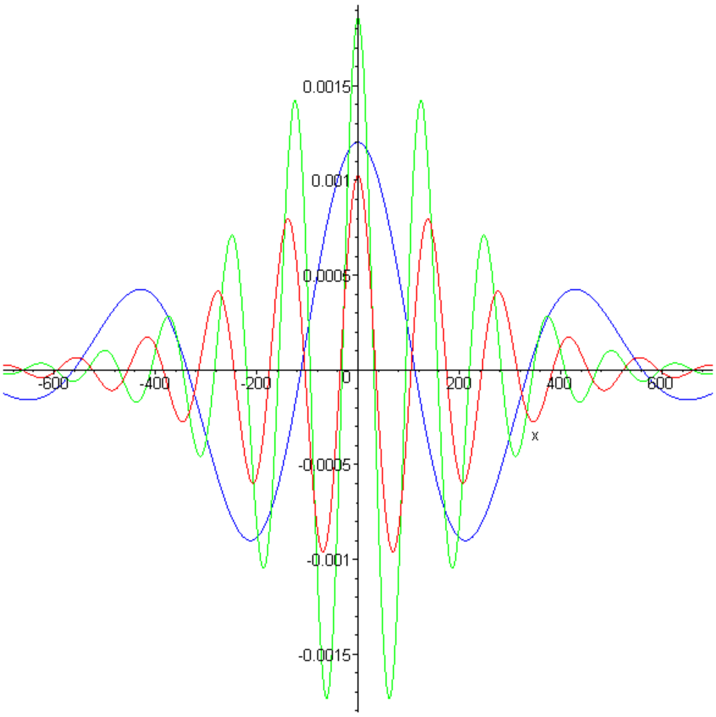


$\alpha = 13$ eV, $\beta = 888$ eV

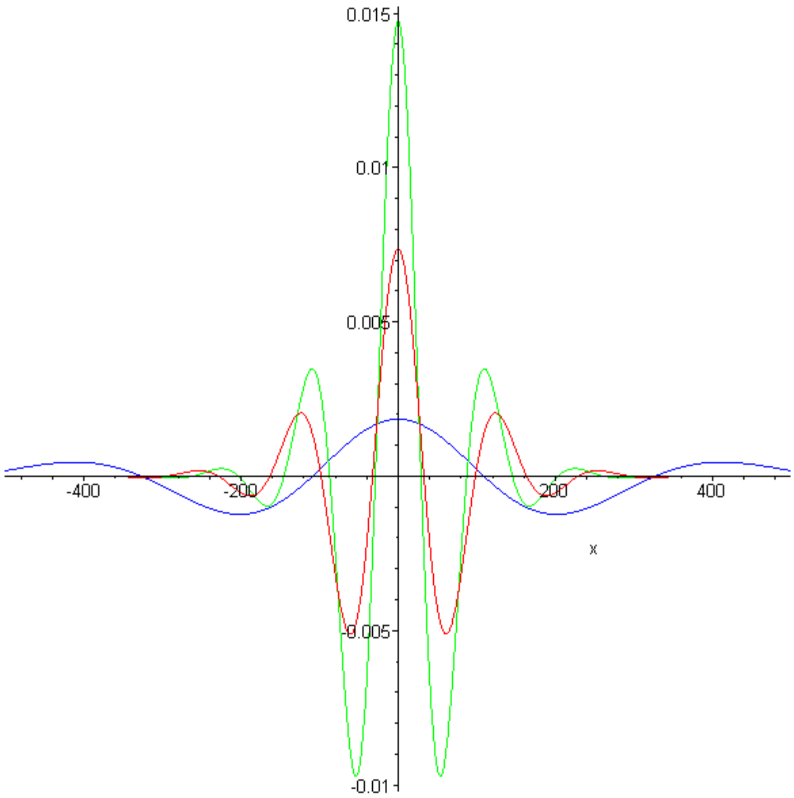


$\alpha = 3.1$ eV, $\beta = 2957$ eV

Fig. 1. The function $\psi(x) = \dfrac{A}{\mathrm{ch}^2 Bx}$ in the range of the negative curvature ($k = \sqrt{\dfrac{\alpha}{8\beta}}$)



a) in the vicinity of the change of the energetic spectrum curvature (etc., in the vicinity of the $k_0 = \pm(\alpha_i / 6\beta_i)^{1/2}$ point)



b) at $k = \sqrt{\dfrac{\alpha}{5\beta}}$

Fig. 2. Function $\psi(x)$ for the different parameters of the dispersion law (1) ($\alpha_1 = 5.7$ eV, $\beta_1 = 479$ eV – *red line*; $\alpha_2 = 13$ eV, $\beta_2 = 888$ eV –*green line*; $\alpha_3 = 3.1$ eV, $\beta_3 = 2957$ eV- *blue line*)

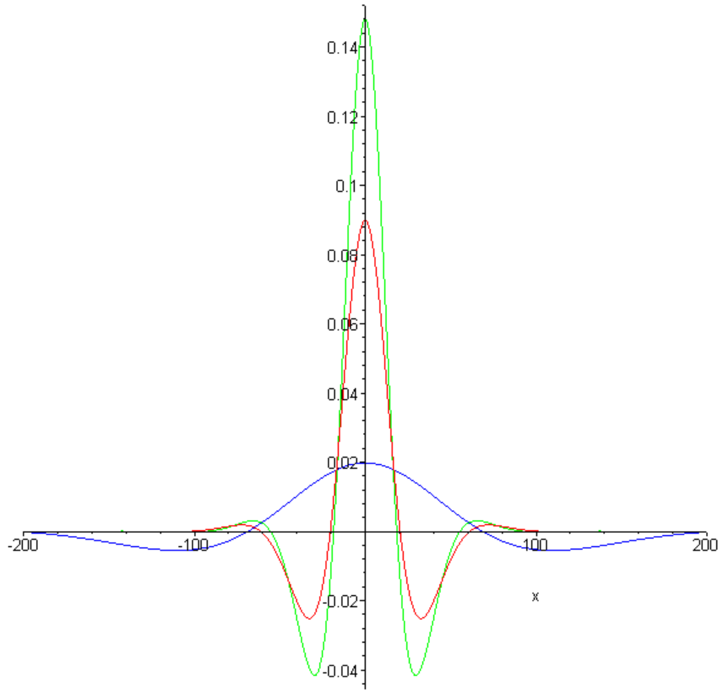
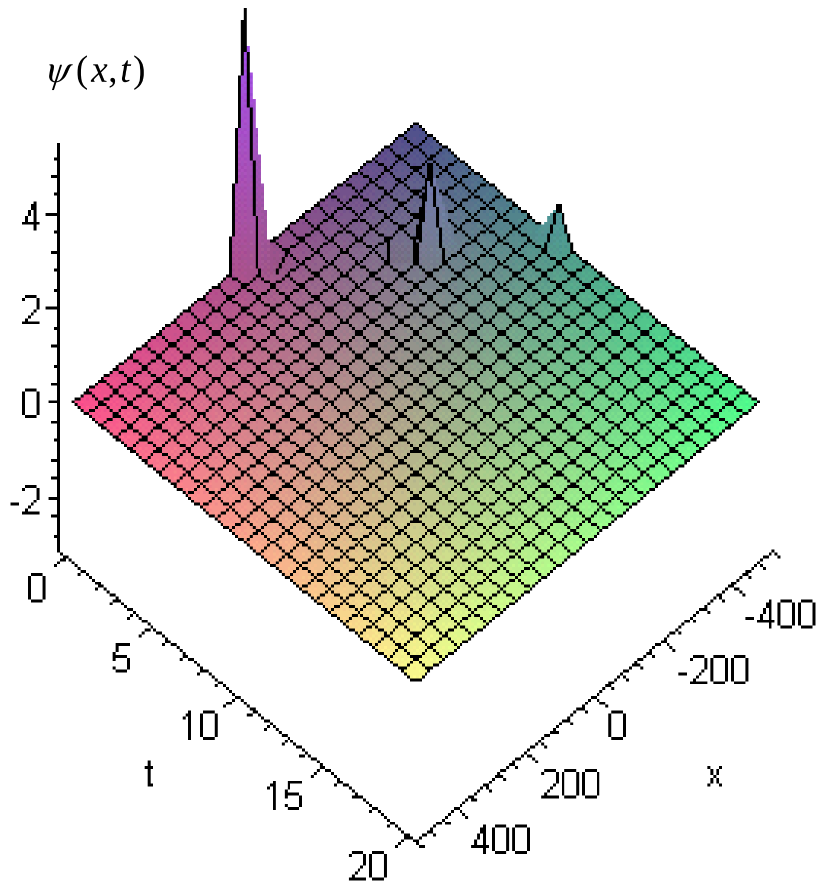
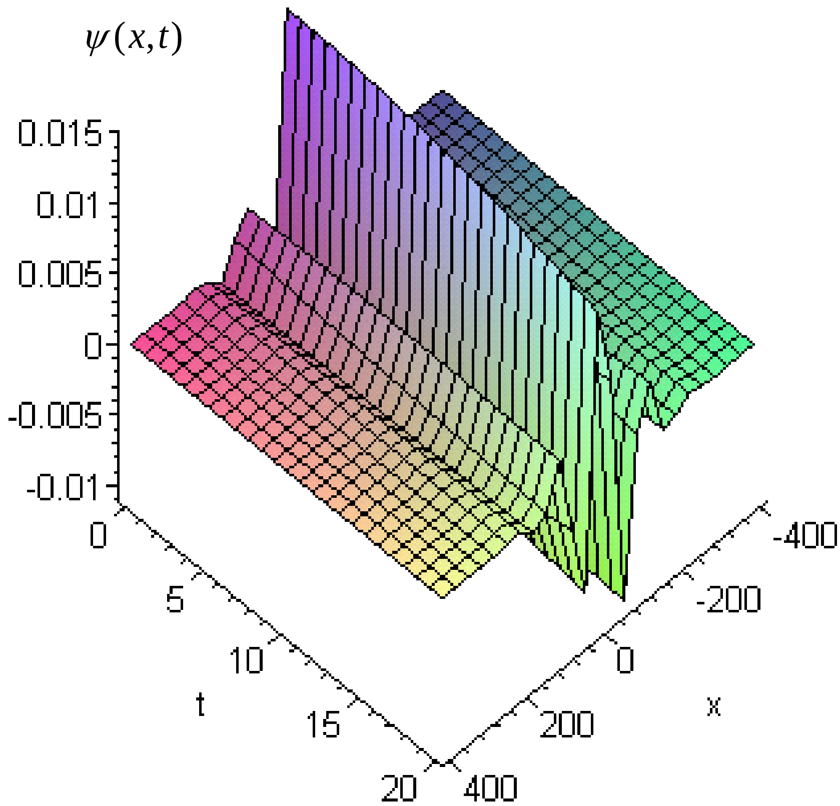


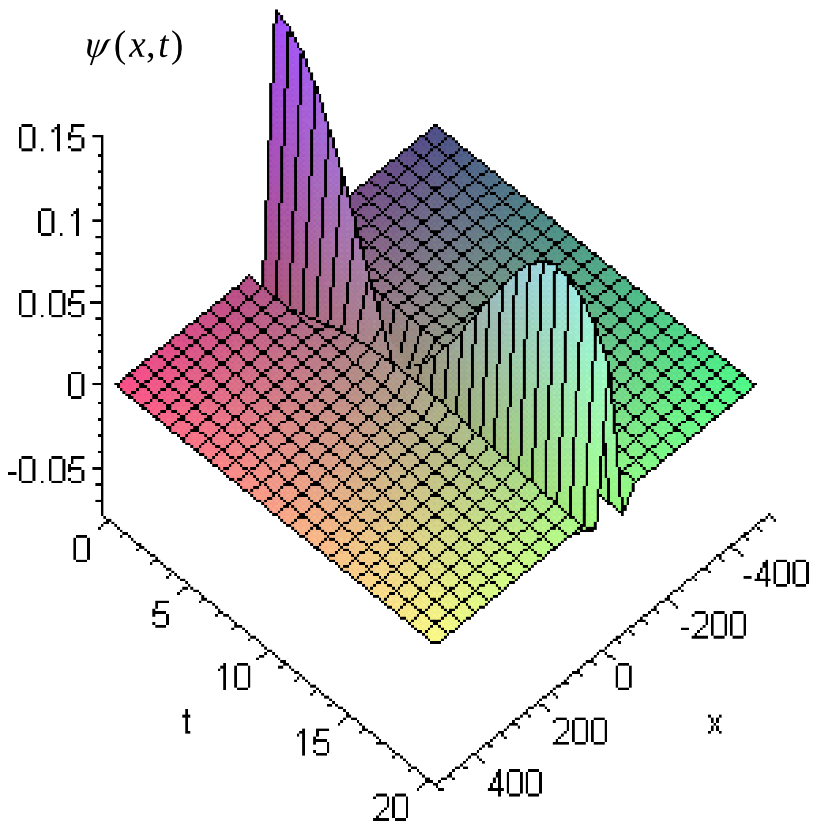
Fig. 3. Function $\psi(x)$ at the different parameters of the dispersion law (1) in the $k=\sqrt{\dfrac{\alpha}{2\beta}}$ point/



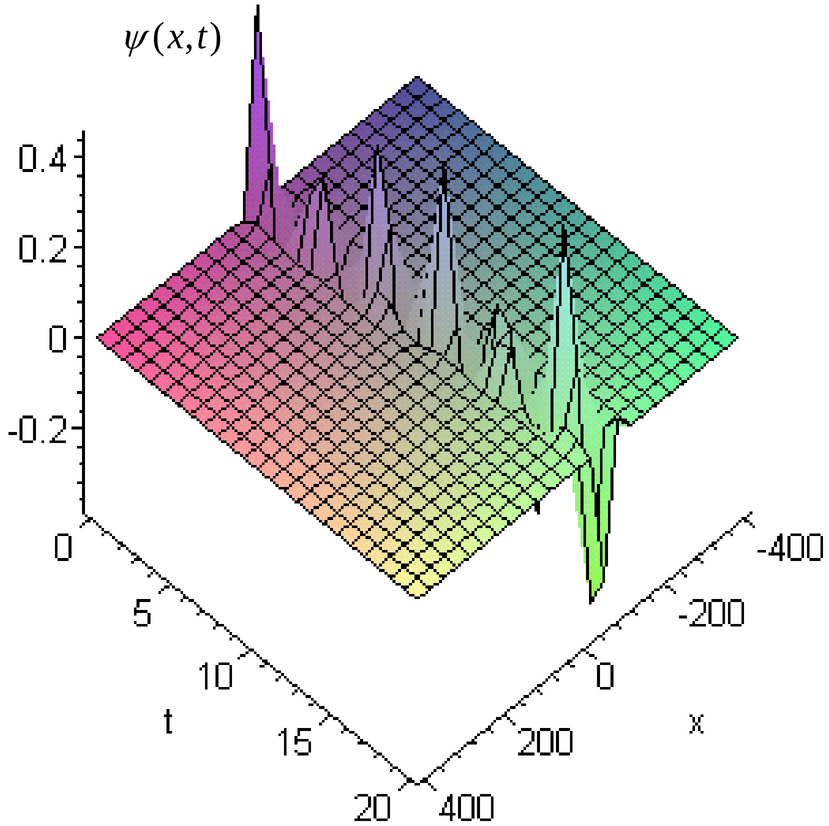
a) $k=\sqrt{\dfrac{\alpha}{8\beta}}$



b) $k = \sqrt{\dfrac{\alpha}{5\beta}}$

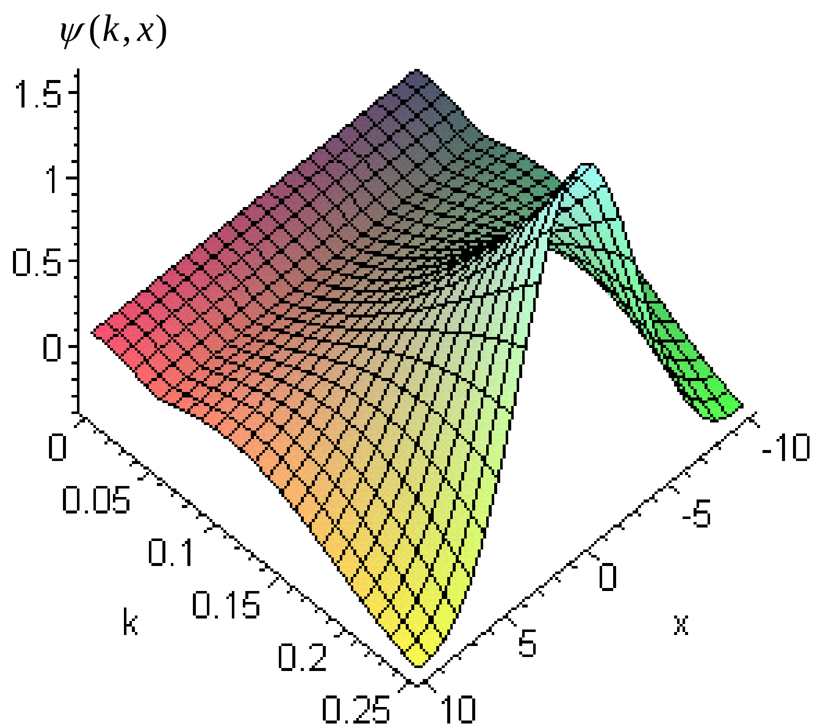


c) $k = \sqrt{\dfrac{\alpha}{2\beta}}$

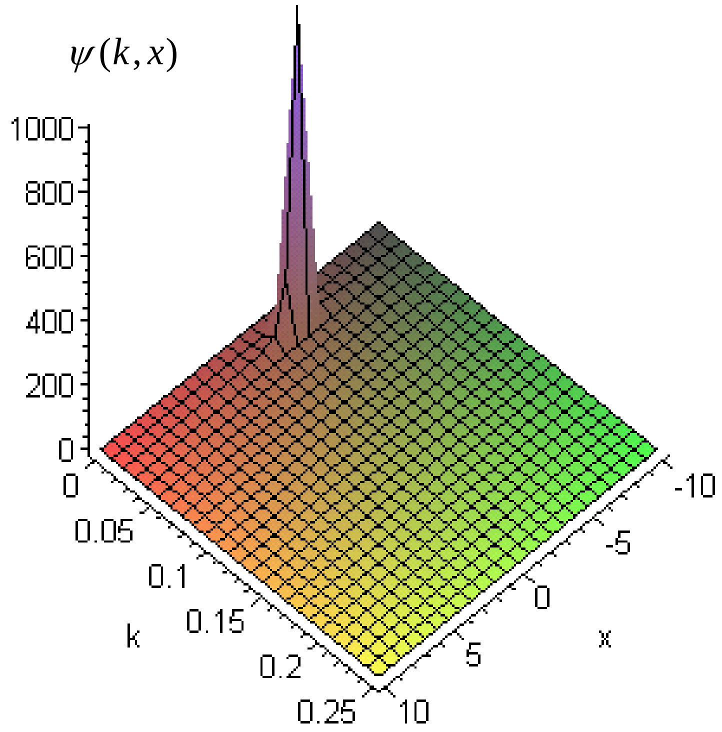


d) $k = \sqrt{\dfrac{\alpha}{\beta}}$

Fig. 4. The function distribution $\psi(x,t)$ at the definite wave vector value.



t=0



t=200

Fig. 5. Function dependence $\psi(k,x)$ on the wave vector ($k=0\div0.25$) at the dispersion law parameters $\alpha_2=13$ eV, $\beta_2=888$ eV.

Conclusion

Thus, the performed numerical investigations of the nonlinear Schrodinger equation with the fourth-order dispersion obtained on the base of the dispersion law with the low-energy non-parabolicity show that the different type of the soliton excitations can be realized in the In_4Se_3 crystal: from one soliton to multisoliton. The theoretical predictions of the stable solitary waves were made for a large number of the variations of the wave vector and the dispersion law parameters.

Since there is a possibility to change these parameters and also the intensity of the electron-phonon interaction by means of the external factors (pressure or impurities) [20, 22, 23], the possibility of the controlled solitary wave's propagation (different width, shape, and height) occurs. It discovers the new perspective applications for the In_4Se_3 crystal, for instance, in the nonlinear optics.

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ОСОБЕННОСТИ СОЛИТОННЫХ ВОЗБУЖДЕНИЙ В КРИСТАЛЛЕ In_4Se_3

Для кристалла In_4Se_3 в рамках нелинейного уравнения Шредингера проведены исследования пространственно -локализованных возбуждений солитонного типа. Показано, что наличие членов пространственной дисперсии четвертого порядка является определяющим для образования уединенных волн в данном кристалле. Баланс между дисперсионными членами четвертого порядка и нелинейностью, обусловленной решеточной деформацией, может приводить к различным пространственно-локализованных возбуждениям в зависимости от параметров закона дисперсии для носителей заряда и области волнового вектора. Определены параметры солитонов (энергия, амплитуда, скорость). Также исследована временная эволюция для данных локализованных возбуждений.
Ключевые слова: Закон дисперсии с низкоэнергетической непараболичностью; Нелинейное уравнение Шредингера с пространственной дисперсией четвертого порядка; Солитон

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ОСОБЛИВОСТІ СОЛІТОННИХ ЗБУДЖЕНЬ В КРИСТАЛІ In_4Se_3

Для кристалу In_4Se_3 в рамках нелінійного рівняння Шредінгера проведено дослідження просторово- локалізованих збуджень солітонного типу. Показано, що наявність членів просторової дисперсії четвертого порядку є визначальною для утворення одиночних хвиль в даному кристалі. Баланс між дисперсійними членами четвертого порядку і нелінійністю, зумовленою гратковою деформацією, може приводити до різних просторово-локалізованих збуджень в залежності від параметрів закону дисперсії для носіїв заряду та області хвильового вектору. Визначені параметри солітонів (енергія, амплітуда, швидкість). Також досліджена часова еволюція для даних локалізованих збуджень.

Ключові слова: Закон дисперсії з низькоенергетичною непараболічністю; Нелінійне рівняння Шредінгера з просторовою дисперсією четвертого порядку; Солітон.