L. BRIZHIK,[1,2] A.P. CHETVERIKOV,[3] W. EBELING,[4] G. RÖPKE,[5] M.G. VELARDE[6,2]

[1] Bogolyubov Institute for Theoretical Physics, Nat. Acad. of Sci. of Ukraine
(14b, Metrolohichna Str., Kyiv 03680, Ukraine; e-mail: brizhik@bitp.kiev.ua)
[2] Wessex Institute of Technology
(Ashurst, Southampton SO40 7AA, UK)
[3] Faculty of Physics, Chernyshevsky State University
(83, Astrakhanskaya Str., Saratov 410012, Russia)
[4] Institut für Physik, Humboldt Universität
(Newtonstrasse 15, Berlin 12489, Germany)
[5] Institut für Physik, Universität Rostock
(Rostock 18051, Germany)
[6] Instituto Pluridisciplinar, Universidad Complutense
(Paseo Juan XXIII, 1, Madrid 28040, Spain)

PACS 71.10.Li, 63.20.Ry, 71.38.Mx

STABILIZING ROLE OF LATTICE ANHARMONICITY IN THE BISOLITON DYNAMICS

We show that, in anharmonic one-dimensional lattices, the pairing of electrons or holes in a localized bisoliton (called also bisolectron) state is possible due to a coupling between the charges and the lattice deformation that can overcome the Coulomb repulsion. We show that bisolitons are dynamically stable up to the sound velocities in lattices with cubic or quartic anharmonicities, and have finite values of energy and momentum in the whole interval of bisoliton velocities up to the sound velocity in the chain. We calculate the bisoliton binding energy and the critical value of Coulomb repulsion at which the bisoliton becomes unstable and decays into two independent electrosolitons. We estimate these energies for chain parameters that are typical of biological macromolecules and some quasi-one-dimensional conducting systems and show that the Coulomb repulsion in such systems is relatively weak as compared with the binding energy. Our analytical results are in a good agreement with the results of numerical simulations in a broad interval of the parameter values.

Keywords: lattice anharmonicity, bisoliton, bisolectron, Coulomb repulsion, electron, hole, exciton, polaron, model Hamiltonian.

1. Introduction

The electron-phonon interaction leads to the lowering of the energy of quasiparticles (electrons, holes, excitons, *etc.*) [1–6]. Depending on the strength of the coupling and the ratio between the Debye energy of phonons and the resonant (exchange) energy in the lattice, a quasiparticle is either in an almost free band state or is trapped in a large polaron or small polaron state [1–6]. For instance, at moderate values of coupling, large polarons correspond to the lowest energy of the system [6]. From the point of view of conducting properties, a large polaron is the most important case, and there is a wide class of crystals, in which large polarons exist. In one-dimensional molecular crystals, such large polarons have been described by a system of nonlinear equations which admit solutions in the form of the so-called Davydov's solitons [6–8]. It has been shown that, in a harmonic lattice, the pairing of two electrons or holes with opposite spins in a bisoliton state takes place [9–11]. Here, we study how the lattice anharmonicity affects the electron pairing in a one-dimensional lattice with account of the Coulomb repulsion. Below, we define the Hamiltonian of the system, which consists of an anharmonic lattice and two extra electrons (or holes) with opposite spins. We derive the corresponding system of equations in the adiabatic approximation for the bisolectron wave function and a lattice deformation. First, we neglect the Coulomb repulsion between the electrons and find analytical solutions in the form of traveling localized structures of the corresponding evolution equations for the case of cubic and quartic anharmonic lattice potentials. Then, us-

ing these solutions, we take the Coulomb repulsion between electrons into account and find conditions for the bisoliton stability with respect to the decay into two isolated solitons.

2. Model Hamiltonian and Dynamic Equations

Let us consider two excess electrons in an infinitely long one-dimensional lattice formed by unit cells of mass M at equilibrium lattice spacing a. Such a system can be described by the Fröhlich Hamiltonian in the form

$$H = H_{\rm el} + H_{\rm lat} + H_{\rm int} + H_{\rm Coul}. \tag{1}$$

Here, the electron Hamiltonian is written as

$$H_{\rm el} = \sum_{n,s} \left[E_0 B^{\dagger}_{n,s} B_{n,s} - J B^{\dagger}_{n,s} \left(B_{n+1,s} + B_{n-1,s}\right)\right], \tag{2}$$

where E_0 is the on-site electron energy, J is the electron exchange interaction energy, and $B^{\dagger}_{n,s}$, and $B_{n,s}$ are the creation and annihilation operators of an electron with spin $s = 1, 2$ on the lattice site n.

The Hamiltonian of the lattice with one phonon mode only has the form

$$H_{\rm ph} = \sum_{n} \left[\frac{\hat{p}_n^2}{2M} + \hat{U}\left(\hat{\beta}_n\right)\right], \tag{3}$$

where $\hat{\beta}_n$ is the operator of a displacement of the n-th unit cell from its equilibrium position, $\hat{p}_n$ is the operator of the canonically conjugated momentum, and $\hat{U}$ is the operator of the potential energy of the lattice, whose properties will be defined below.

The Hamiltonian of the electron-lattice interaction in the case where the on-site electron energy dependence on the longitudinal displacements of unit cells (acoustical mode) dominates the intersite dependence is given by the expression

$$H_{\rm int} = \chi \sum_{n,s=1,2} \left(\hat{\beta}_{n+1} - \hat{\beta}_{n-1}\right) B^{\dagger}_{n,s} B_{n,s}, \tag{4}$$

where χ is the electron-lattice coupling constant.

The Coulomb repulsion between the electrons is given by the Hubbard-type Hamiltonian

$$H_{\rm Coul} = \sum_{n,m,s=1,2} V_{nm} B^{\dagger}_{n,s} B_{n,s} B^{\dagger}_{m,s} B_{m,s}, \tag{5}$$

where V_{nm} is the corresponding matrix element of the Coulomb interaction.

In the adiabatic approximation, we can set

$$|\Psi(t)\rangle = |\Psi_{\rm el}(t)\rangle |\Psi_{\rm ph}(t)\rangle. \tag{6}$$

Here, the vector state of the lattice has the form of the product of the operator of coherent displacements of unit cells and the vacuum state of the lattice, $|0\rangle_{\rm ph}$,

$$|\Psi_{\rm ph}(t)\rangle = \exp\left\{-\frac{i}{\hbar}\sum_{n}\left[\beta_n(t)\hat{p}_n - p_n(t)\hat{\beta}_n\right]\right\}|0\rangle_{\rm ph}, \tag{7}$$

where $\beta_n(t)$ and $p_n(t)$ are, respectively, the mean values of the displacements of unit cells from their equilibrium positions and their canonically conjugated momenta in state (6).

The electron state vector for two excess electrons has the form

$$|\Psi_{\rm el}(t)\rangle = \sum_{n_1,n_2,s_1,s_2} \Psi(n_1,n_2,s_1,s_2;t) B^{\dagger}_{n_1,s_1} B^{\dagger}_{n_2,s_2} |0\rangle_{\rm el}. \tag{8}$$

In the absence of a magnetic field, we can represent the singlet electron function $\Psi(n_1,n_2,s_1,s_2;t)$ for two electrons with antiparallel spins as the product of the symmetric coordinate function $\Psi(n_1,n_2,t)$ and the antisymmetric spin function $\chi(s_1,s_2)$. Using such a state vector, we can calculate the Hamiltonian functional $\mathcal{H} = \langle\Psi(t)|H|\Psi(t)\rangle$, corresponding to the Hamiltonian operator (1).

We are interested in functions slowly varying in space that correspond to solutions of the soliton class. Therefore, we can use the continuum approximation $n \to x \equiv na$. Minimizing the functional $\mathcal{H}$ with respect to electron and phonon variables and neglecting the Coulomb repulsion, we derive the system of equations

$$-i\hbar\frac{\partial\Psi}{\partial t} - \frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x_1^2} + \frac{\partial^2\Psi}{\partial x_2^2}\right) = \\ = \chi a\left(\frac{\partial\beta(x,t)}{\partial x}\bigg|_{x=x_1} + \frac{\partial\beta(x,t)}{\partial x}\bigg|_{x=x_2}\right)\Psi, \tag{9}$$

$$\frac{\partial^2\beta}{\partial t^2} - V_{\rm ac}^2\frac{\partial^2 U}{\partial\rho^2}\frac{\partial^2\beta}{\partial x^2} - \alpha\frac{\partial^4\beta}{\partial x^2\partial t^2} = \\ = \frac{a}{M}\chi\left(\int dx_2 \frac{\partial|\Psi|^2}{\partial x_1}\bigg|_{x_1=x} + \int dx_1 \frac{\partial|\Psi|^2}{\partial x_2}\bigg|_{x_2=x}\right). \tag{10}$$

Here, $\rho(x,t) = -\partial\beta(x,t)/\partial x$ is the local deformation of the lattice, and V_{ac} is the linear sound velocity in the chain. On the left-hand side of the latter equation, we have included an extra term proportional to the fourth derivative of the lattice displacement to take a nonlinear dispersion of the lattice into account, if any (see, e.g., comments in [12]).

The potential energy of the lattice $U(\rho)$ has a minimum in the equilibrium lattice. We assume that it is increasing with the electron-induced compression of the lattice ($\rho > 0$) (see [12–14]):

$$\frac{\partial U(\rho)}{\partial \rho}|_{\rho=0} = 0, \quad \frac{\partial^2 U(\rho)}{\partial \rho^2} > 0. \tag{11}$$

The two-electron wave function can be represented as the symmetrized product of 'one-electron' wave functions. Introducing the running wave coordinate $\xi = (x - x_0 - Vt)/a$, we can rewrite the system of equations in the following form:

$$\frac{d^2\Phi_j}{d\xi^2} + \sigma\rho\Phi_j = \lambda_j\Phi_j, \quad j = 1,2, \tag{12}$$

$$\frac{dF}{d\rho} = D(\Phi_1^2 + \Phi_2^2), \tag{13}$$

where F is the effective lattice potential

$$F = U(\rho) - \frac{1}{2}s^2\rho^2, \quad s^2 = \frac{V^2}{V_{ac}^2}, \tag{14}$$

and the following dimensionless parameters are introduced:

$$\lambda_j = -\frac{E_j}{J}, \quad \sigma = \frac{\chi a}{J}, \quad D = \frac{\chi a}{MV_{ac}^2}, \tag{15}$$

with E_j being the electron eigenenergy, and Φ_j being the envelope function of the corresponding 'one-electron' wave functions Ψ_j in the two-electron state.

We can rewrite Eq. (12) in the form

$$\left(\frac{d\Phi_j}{d\xi}\right)^2 = \lambda_j\Phi_j^2 - \sigma Q_j, \tag{16}$$

where the notation

$$Q_j(\xi) = \int\limits_{-\infty}^{\xi} \rho(x)d\Phi_j^2(x), \quad j = 1,2, \tag{17}$$

is introduced. For localized solutions, the corresponding functions attain some maximum values denoted as $\Phi_{j,0}$ and ρ_0, respectively. In one-dimensional systems, the deformational potential has at least one bound state, which can be occupied by two electrons with opposite spins. When the Coulomb repulsion is very weak, the minimum energy state corresponds to the case where the maxima of 'one-electron' functions coincide [9–11] and

$$\lambda_1 = \lambda_2, \qquad \Phi_1(\xi) = \Phi_2(\xi). \tag{18}$$

Therefore, we can omit index j in what follows.

In the general case, the maximum values of the 'one-electron' wave functions are shifted along the lattice by some value l_0 due to the Coulomb repulsion, which will be considered in the corresponding section below.

From Eq. (16), we obtain the expression for the electron eigenenergies:

$$\lambda = \sigma\frac{Q(0)}{\Phi_0^2}. \tag{19}$$

From Eq. (13), we get the equation which determines the lattice deformation

$$\frac{d\rho}{d\xi} = \pm 2\frac{dF/d\rho}{d^2F/d\rho^2}\sqrt{\lambda - \sigma G(\rho)}, \tag{20}$$

where

$$G(\rho) = \rho - \frac{F(\rho)}{dF/d\rho} \tag{21}$$

and

$$\lambda = \sigma G(\rho_0). \tag{22}$$

Integrating Eq. (20), we get

$$\xi(\rho) = \pm\frac{1}{2\sqrt{\sigma}}\int\limits_{\rho(\xi)}^{\rho_0} \frac{d^2F/d\rho^2}{dF/d\rho}\frac{1}{\sqrt{G(\rho_0) - G(\rho)}}d\rho. \tag{23}$$

From the normalization condition for 'one-electron' wave functions, we find the expression for their maximum

$$\Phi_0 = \sqrt{\frac{1}{2D}\left(\frac{dF}{d\rho}\right)\Big|_{\rho=\rho_0} G(\rho_0)}. \tag{24}$$

To get the explicit solutions, we have to specify the lattice potential. Below, we will consider two cases

of cubic and quartic anharmonic potentials. Respectively, we assign subscript 'c' or 'q' to the functions:

$$U_c(\rho) = \frac{1}{2}\rho^2 + \frac{\alpha}{3}\rho^3, \quad U_q(\rho) = \frac{1}{2}\rho^2 + \frac{\beta}{4}\rho^4. \tag{25}$$

Substituting these expressions into Eq. (14), we get

$$F_c(\rho) = \frac{\alpha}{2}\rho^2\left(\frac{2}{3}\rho + \delta_c\right), \quad F_q(\rho) = \frac{\beta}{4}\rho^2\left(\rho^2 + 2\delta_q\right). \tag{26}$$

From Eq.(21), we find

$$G_c = \frac{\rho}{6}\frac{4\rho + 3\delta_c}{\rho + \delta_c}, \quad G_q = \frac{\rho}{4}\frac{3\rho^2 + 2\delta_q}{\rho^2 + \delta_q}, \tag{27}$$

where the dynamically modulated inverse anharmonic stiffness coefficients are introduced as

$$\delta_c = \frac{1 - s^2}{\alpha}, \quad \delta_q = \frac{1 - s^2}{\beta}. \tag{28}$$

Substituting the explicit form of G into Eq. (23), we can rewrite the expression in the form

$$\xi_\nu(\rho) = \pm\frac{1}{2\sqrt{\sigma}}\int\limits_{\rho(\xi)}^{\rho_{0(\nu)}} \frac{K_\nu(\rho, \rho_{0(\nu)})}{\rho\sqrt{\rho_{0(\nu)} - \rho}}d\rho, \quad \nu = c, q, \tag{29}$$

where the kernel of the integral for both types of anharmonic potentials K_ν in view of the explicit form of G_ν is very close to unity (see the numerical solution in [15, 16]). From Eq. (29) after the integration, we find that the deformation of the lattice is given by the soliton solutions of the B-KdV equation [6, 17–23] and the Zakharov–Davydov system of nonlinear equations [6, 8]:

$$\rho_\nu(\xi) = \rho_{0(\nu)}\mathrm{Sech}^2(\kappa_\nu\xi), \tag{30}$$

the width of which, κ, is determined by the maximum value of the deformation

$$\kappa_c = \sqrt{\frac{\sigma\rho_{0(c)}}{2}}\frac{\sqrt{4\rho_{0(c)}\left(\rho_{0(c)} + 2\delta_c\right)/3 + \delta_c^2}}{2\rho_{0(c)} + \delta_c}, \tag{31}$$

$$\kappa_q = \frac{1}{2}\sqrt{\frac{\sigma\rho_{0(q)}\left(3\rho_{0(q)}^2 + 2\delta_q\right)}{\rho_{0(q)}^2 + 2\delta_q}}, \tag{32}$$

which can be approximated by the expression

$$\kappa_\nu \approx \sqrt{\frac{\sigma\rho_{0(\nu)}}{2}}. \tag{33}$$

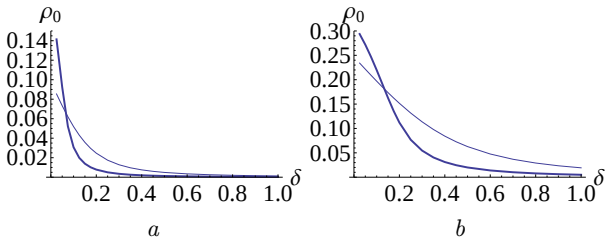

Fig. 1. Maximum value of the lattice deformation as a function of the dynamically modulated inverse anharmonic stiffness coefficient δ in lattices with cubic (thin line) and quartic (thick line) anharmonicities for g_ν=0.05 (a) and g_ν=0.2 (b)

In its turn, $\rho_{0(\nu)}$ is determined by the corresponding equation

$$\rho_{0(c)}\left(\frac{4}{3}\rho_{0(c)} + \delta_c\right)^2 = g_c^2\theta_c(\rho_{0(c)}), \tag{34}$$

$$\rho_{0(q)}\left(\frac{8}{5}\rho_{0(q)}^2 + \delta_q\right)^2 = g_q^2\theta_q(\rho_{0(q)}), \tag{35}$$

where g_ν is a constant determined below,

$$g_c^2 = \frac{D^2\sigma}{\alpha^2}, \quad g_q^2 = \frac{D^2\sigma}{\beta^2}, \tag{36}$$

and the following notations are introduced:

$$\theta_c(\rho_{0(c)}) = \frac{4\rho_{0(c)}(\rho_{0(c)} + 2\delta_c) + 3\delta_c^2}{6(\rho_{0(c)} + \delta_c)^2}, \tag{37}$$

$$\theta_q(\rho_{0(q)}) = \frac{3\rho_{0(q)}^4 + 7\delta_q\rho_{0(q)}^2 + 2\delta_q^2}{4\left(\rho_{0(q)}^2 + \delta_q\right)^2}. \tag{38}$$

The numerical solutions of Eqs. (34) and (35) are shown in Fig. 1 for two different values of the coupling constant.

It follows from Fig. 1 that (i) the maximum lattice deformation depends on the soliton velocity; (ii) the soliton amplitude increases, and its width decreases, as the velocity increases, and attain some finite values at the sound velocity, $V = V_{ac}$ (*i.e.*, $\delta = 0$); (iii) the soliton amplitude increases with the electron-lattice coupling; (iv) the quartic anharmonicity is dominant at small values of δ (large velocities), while the cubic anharmonicity is dominant at larger values of δ (small velocities).

From Eqs. (13), we obtain

$$\Phi^2(\xi) = \frac{1}{2D}\frac{dF(\rho)}{d\rho}. \tag{39}$$

Using the explicit expression for F from Eq. (26), we find the electron wave function

$$\Phi_c(\xi) = \sqrt{\frac{\rho_{0(c)}}{2D}}\mathrm{Sech}(\kappa_c\xi) \times$$
$$\times\sqrt{1 - s^2 + \alpha\rho_{0(c)}\mathrm{Sech}^2(\kappa_c\xi)}, \quad (40)$$
$$\Phi_q(\xi) = \sqrt{\frac{\rho_{0(q)}}{2D}}\mathrm{Sech}(\kappa_c\xi) \times$$
$$\times\sqrt{1 - s^2 + \beta\rho^2_{0(q)}\mathrm{Sech}^4(\kappa_q\xi)}. \quad (41)$$

Finally, we write down the energy and the momentum of the system described by Hamiltonian (1)–(4) in the bisolectron state (6)–(8):

$$E^{(\mathrm{bs})}_{\mathrm{tot}}(V) = mV^2 + E^{(bs)}(V) + W(V), \quad (42)$$

$$P_{(\mathrm{bs})}(V) = \left[2m + M\sqrt{\frac{2}{\sigma}}\int\limits_0^{\rho_0} K(\rho,\rho_o)\frac{\rho}{\sqrt{\rho_0-\rho}}d\rho\right]V \approx$$
$$\approx \left[2m + \frac{4}{3}M\sqrt{\frac{2}{\sigma}}\rho_0^{3/2}\right]V. \quad (43)$$

Here, we reckon the energy from the electron energy E_0, $m = \hbar^2/(2Ja^2)$ is the effective band mass of an electron, $E^{(\mathrm{bs})}(V) = -2\lambda J$ is the bisoliton energy, and W is the energy of the lattice deformation:

$$W(V) = 2MV^2_{ac}\int\limits_{-\infty}^{0}\left(F(\rho) + s^2\rho^2\right)d\xi, \quad (44)$$

or, in terms of the F and G functions given by expressions (14), (21), respectively:

$$E^{(\mathrm{bs})}(V) = -2DG(\rho_0)MV^2_{ac}, \quad (45)$$

$$W(V) = \frac{MV^2_{ac}}{\sqrt{\sigma}}\int\limits_0^{\rho_0}\frac{d^2F/d\rho^2}{dF/d\rho}\frac{F(\rho)+s^2\rho^2}{\sqrt{G(\rho_0)-G(\rho)}}\,d\rho. \quad (46)$$

Using now the bisolectron solutions (30) and (40) for the cubic anharmonicity, we obtain

$$E^{(\mathrm{bs})}_c(V) = -DMV^2_{ac}\rho_{0(c)}\frac{4\rho_{0(c)}+3\delta_c}{3(\rho_{0(c)}+\delta_c)}, \quad (47)$$

$$W_c(V) \approx \frac{MV^2_{ac}}{3\sqrt{2\sigma}}\rho^{3/2}_{0(c)}\left(\frac{8}{15}\alpha\rho_{0(c)} + 1 + s^2\right). \quad (48)$$

For solutions (30) and (41) in a quartic anharmonic lattice, we have

$$E^{(\mathrm{bs})}_q(V) = -\frac{1}{2}DMV^2_{ac}\rho_{0(q)}\frac{3\rho^3_{0(q)}+2\delta_q}{\rho^2_{0(q)}+\delta_q}, \quad (49)$$

$$W_q(V) \approx 8\frac{MV^2_{ac}}{\sqrt{2\sigma}}\rho^{3/2}_{0(q)}\left[\frac{1}{3}\left(s^2 + \frac{1}{2}\delta\beta\right) + \frac{2}{35}\beta\rho^2_{0(q)}\right]. \quad (50)$$

Two important conclusions follow from the above expressions. First of all, comparing the bisolectron energies with the energies of solectrons (see [12–14]), we conclude that there is the positive binding energy of a bisolectron in the whole interval of velocities $V^2 \le V^2_{ac}$

$$E^{(\mathrm{bs})}_{\mathrm{bind}(\nu)}(V) = 2E^{(\mathrm{s})}_{\mathrm{tot}(\nu)}(V) - E^{(\mathrm{bs})}_{\mathrm{tot}(\nu)}(V), \quad \nu = c, q, \quad (51)$$

which means that an anharmonic lattice soliton can capture two electrons with opposite spins, and such a bisolectron state is energetically favorable as comparing with two independent solectrons (lattice soliton bound with one electron). Here, $E^{(\mathrm{bs})}_{\mathrm{tot}(\nu)}(V)$ is the total energy of the system in the bisolectron state with account of the energy of the lattice deformation, and $E^{(\mathrm{s})}_{\mathrm{tot}(\nu)}(V)$ is the energy of the system with one electron in a soliton state with account of the energy of the lattice deformation.

Second, we see that the bisolectron energy and the energy of the lattice deformation take finite values at the velocity of the bisolectron equal to the velocity of the sound in the chain, namely:

$$E^{(\mathrm{bs})}_{\mathrm{tot(c)}}(V_{ac}) = mV^2_{ac} - \frac{2}{3}\chi a\rho_{0(c)} + \frac{16}{45}\chi a\alpha\rho^2_{0(c)}, \quad (52)$$

$$E^{(\mathrm{bs})}_{\mathrm{tot(q)}}(V_{ac}) = mV^2_{ac} - \frac{3}{2}\chi a\rho^2_{0(q)} + \frac{8}{35}\chi a\beta\rho^3_{0(q)}. \quad (53)$$

At small velocities, the bisolectron energy increases with the velocity, according to the law

$$E^{(\mathrm{bs})}_{\mathrm{tot(c)}}(V) = mV^2 -$$
$$-\frac{1}{3}\chi a\rho_{0(c)}\left(1 - 2s^2 - \frac{1}{15}\alpha\rho_{0(c)} + 7\alpha\rho_{0(c)}s^2\right), \quad (54)$$
$$E^{(\mathrm{bs})}_{\mathrm{tot(q)}}(V_{ac}) = mV^2 -$$

$$-\frac{1}{3}\chi a\rho_{0(q)}\left(1-2s^2+3\beta\rho_{0(q)}^2s^2-\frac{129}{35}\beta\rho_{0(q)}^2\right). \quad (55)$$

From the above two equations, we can calculate the bisolectron band bottom energy level and the bisolectron effective mass in the effective mass approximation:

$$E_{0(c)}^{(\mathrm{bs})}=-\frac{2}{3}Jg^2\left(1-\frac{1}{15}\alpha\frac{2Jg^2}{\chi a}\right), \quad (56)$$

$$M_c^{(\mathrm{bs})}=2m+\frac{4}{3}\frac{Jg^2}{V_{ac}^2}\left(1-7\alpha\frac{Jg^2}{\chi a}\right), \quad (57)$$

$$E_{0(q)}^{(\mathrm{bs})}=-\frac{2}{3}Jg^2\left(1-\frac{129}{35}\beta 4g^2\frac{J^2}{\chi^2a^2}\right), \quad (58)$$

$$M_q^{(\mathrm{bs})}=2m+\frac{4}{3}\frac{Jg^2}{V_{ac}^2}\left(1-6\beta\frac{J^2g^4}{\chi^2a^2}\right). \quad (59)$$

Here, g is the dimensionless electron-lattice coupling constant,

$$g\equiv\frac{\chi^2}{2Jw}. \quad (60)$$

3. Bisolectron with Account of the Coulomb Repulsion

Let us now take into account the Coulomb repulsion between the electrons. The total energy of system (42) in the bisolectron state with account of the Coulomb repulsion is

$$\mathcal{E}_{\mathrm{tot}(\nu)}^{(\mathrm{bs})}(V)=E_{\mathrm{tot}(\nu)}^{(\mathrm{bs})}(V)+E_{\mathrm{Coul}}. \quad (61)$$

In the systems, whose parameters satisfy the condition of the adiabatic approximation (intermediate value of the electron-lattice coupling and a relatively small non-adiabaticity parameter), a bisolectron is extended over a few lattice sites. Therefore, the energy of the Coulomb repulsion can be written as

$$E_{\mathrm{Coul}}\approx\frac{e^2}{4\pi\epsilon la}, \quad (62)$$

where e is the effective electron charge with account of its screening in the lattice due to the surrounding and the complex structure of a unit site, and $\epsilon=\epsilon_{\mathrm{m}}\epsilon_0$ is the dielectric constant of the lattice, which contains the dielectric constant ϵ_{m} of the medium.

Above, we have obtained the soliton solutions for two electrons with antiparallel spins, bound with the lattice soliton, in the approximation of a very weak Coulomb repulsion. In such a case, both 'one-electron' wave functions have maximum values at the same position in the lattice. In the general case, the corresponding maximum values are shifted along the lattice by some value l_0, which is determined by the balance between the Coulomb repulsion between the electrons and their attraction due to the interaction with the lattice:

$$\Phi_j(\xi)=\Phi_j(\xi\pm l_0/2)f_j(l_0), \quad (63)$$

where $f_j(l_0)$ takes into account the change of the 'one-electron' wave functions due to the Coulomb repulsion. For localized states extended over few lattice sites, the repulsion is expected to be weak: $f_j(l_0)\approx\approx 1+\varepsilon(l_0)$, where $\varepsilon\ll 1$ is a smallness parameter. Therefore, in the lowest order approximation with respect to ε, the maxima of 'one-electron' functions coincide at $\xi=0$, as was considered in the previous section.

According to Eq. (63),we have the following expressions for the wave functions for the cubic anharmonicity in the presence of the Coulomb repulsion (see (40)):

$$\Phi_{j(c)}(\xi)=\sqrt{\frac{\rho_{0(c)}}{2D}}\mathrm{Sech}\left(\kappa_c(\xi\pm\frac{l}{2})\right)\times$$
$$\times\sqrt{1-s^2+\alpha\rho_{0(c)}\mathrm{Sech}^2\left(\kappa_c(\xi\pm\frac{l}{2})\right)}. \quad (64)$$

For a lattice with quartic anharmonicity (see (41)), we have

$$\Phi_{j(q)}(\xi)=\sqrt{\frac{\rho_{0(q)}}{2D}}\mathrm{Sech}\left(\kappa_q(\xi\pm\frac{l}{2})\right)\times$$
$$\times\sqrt{1-s^2+\beta\rho_{0(q)}^2\mathrm{Sech}^4\left(\kappa_q(\xi\pm\frac{l}{2})\right)}. \quad (65)$$

The distance between the maxima of the 'one-electron' wave functions, l, can be determined from the condition of the minimum of the total energy of the system with account of the Coulomb repulsion. To calculate it, let us consider, for simplicity, the case of a bisolectron at rest, $V=0$. Substituting function (64) (or (65)) and the corresponding lattice deformation (30) into the Hamiltonian $\mathcal{H}$ and expanding the result with respect to l in the assumption $l<\mu=2\pi/\kappa_\nu$, we obtain, after the integration,

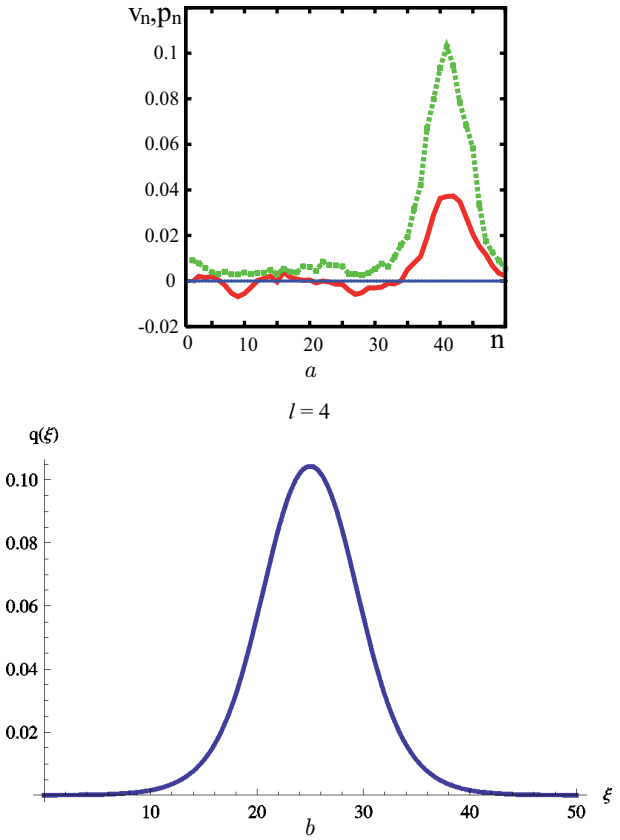

Fig. 2. Results of numerical simulations for the electron density (green dashed line) and the velocity distribution (red solid line) at $\bar{U} = 20$ (a). Blue curve corresponds to bisolectron density profile $q(x)$ is based on the analytical results (64) at $l = l_0 = 4$ (b)

the total energy of the system including the Coulomb repulsion (62):

$$\mathcal{E}^{(\mathrm{bs})}_{\mathrm{tot}(\nu)}(0) = \frac{2}{3}J\frac{\kappa_\nu}{D}\rho_{0(\nu)} - \frac{4}{3}\frac{\chi a}{\kappa_\nu D}\rho^2_{0(\nu)}\left(1 - l^2\kappa^2_\nu\right) + \\ + wa^2\rho^2_{0(\nu)}\left[\frac{2}{3} + \frac{1}{2}\varsigma_\nu\rho^2_{0(\nu)} - l^2\kappa^2_\nu\left(\frac{1}{3} + \frac{1}{2}\varsigma_\nu\rho^2_{0(\nu)}\right)\right] + \\ + \frac{e^2}{4\pi\epsilon la}, \tag{66}$$

where $\varsigma_c \equiv \alpha$, $\varsigma_q \equiv \beta$, and the energies are counted from the energy of the electron band bottom E_0. Expression (45) can be represented in the general form

$$\mathcal{E}^{(\mathrm{bs})}_{\mathrm{tot}(\nu)}(0) = E^{(\mathrm{bs})}_{\mathrm{tot}(\nu)}(0) + \frac{1}{2}\zeta_\nu l^2 + \frac{e^2}{4\pi\epsilon la}, \tag{67}$$

where the first term is the bisolectron energy in the absence of the Coulomb repulsion, the second term is due to a modification of the wave functions, and the last term is the Coulomb repulsion.

Minimizing this expression with respect to l, we get the equilibrium distance between the maxima of the one-electron functions:

$$l_0 = \left(\frac{e^2}{4\pi\epsilon a\zeta_\nu}\right)^{1/3}, \tag{68}$$

where we used the notation

$$\zeta_q = \left[\frac{4}{3}\frac{\chi a\rho^2_{0(q)}\kappa_q}{D} - wa^2\rho^2_{0(q)}\kappa^2_q\left(\frac{1}{3} + \frac{1}{2}\beta\rho^2_{0(q)}\right)\right]. \tag{69}$$

Expression (68) can be approximated as

$$l_{0(\nu)} = \left(\frac{3De^2}{4\pi\epsilon\chi a^2\rho^2_{0(\nu)}\kappa_\nu}\right)^{1/3}. \tag{70}$$

Substituting these results into Eq. (61), we obtain the final expression for the total energy of the system at $V = 0$

$$\mathcal{E}^{(\mathrm{bs})}_{\mathrm{tot}(\nu)}(0) = E^{(\mathrm{bs})}_{\mathrm{tot}(\nu)}(0) + \frac{3}{2}\left(\frac{e^2}{4\pi\epsilon a}\right)^{2/3}\zeta^{1/3}_\nu + \frac{e^2}{4\pi\epsilon l_0 a}. \tag{71}$$

Here, l_0 is given by Eq. (70).

Such a state is stable with respect to the decay of the bisolectron into two solectrons, if the bisolectron binding energy $\mathcal{E}^{(\mathrm{bs})}_{\mathrm{bind}(\nu)}(0)$ is positive,

$$\mathcal{E}^{(\mathrm{bs})}_{\mathrm{bind}(\nu)}(0) \equiv 2\mathcal{E}^{(\mathrm{s})}_{\mathrm{tot}(\nu)}(0) - \mathcal{E}^{(\mathrm{bs})}_{\mathrm{tot(nu)}}(0) > 0, \tag{72}$$

i.e., when the inequality

$$2E^{(\mathrm{s})}_{\mathrm{tot}(\nu)}(0) - E^{(\mathrm{bs})}_{\mathrm{tot(nu)}}(0) + \frac{3}{2}\left(\frac{e^2}{4\pi\epsilon a}\right)^{2/3}\zeta^{1/3}_\nu > 0 \tag{73}$$

is valid.

4. Comparison with the Numerical Simulations

In this section, we compare the above-obtained analytical results with the numerical results in [26,29] for a discrete lattice with the Morse interaction with two added electrons, described by the Hubbard Hamiltonian. The Morse potential

$$U^{\mathrm{Morse}}(r) = D[(1 - e^{-B(r-a)})^2 - 1]. \tag{74}$$

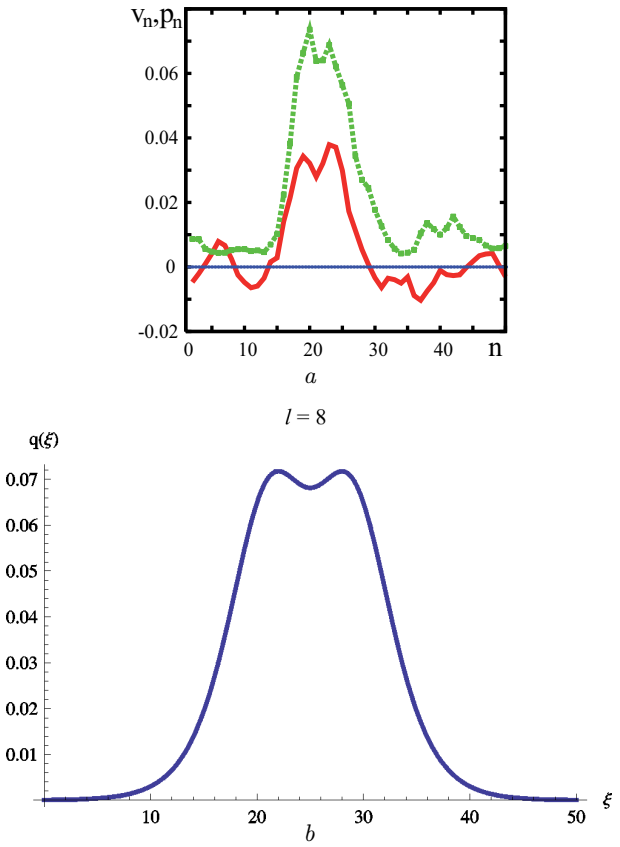

Fig. 3. Results of numerical simulations for the electron density (green dashed line) and the velocity distribution (red solid line) at $\bar{U} = 60$ (a). Blue curve corresponds to bisolectron density profile $q(x)$ is based on the analytical results (64) at $l = l_0 = 8$ (b)

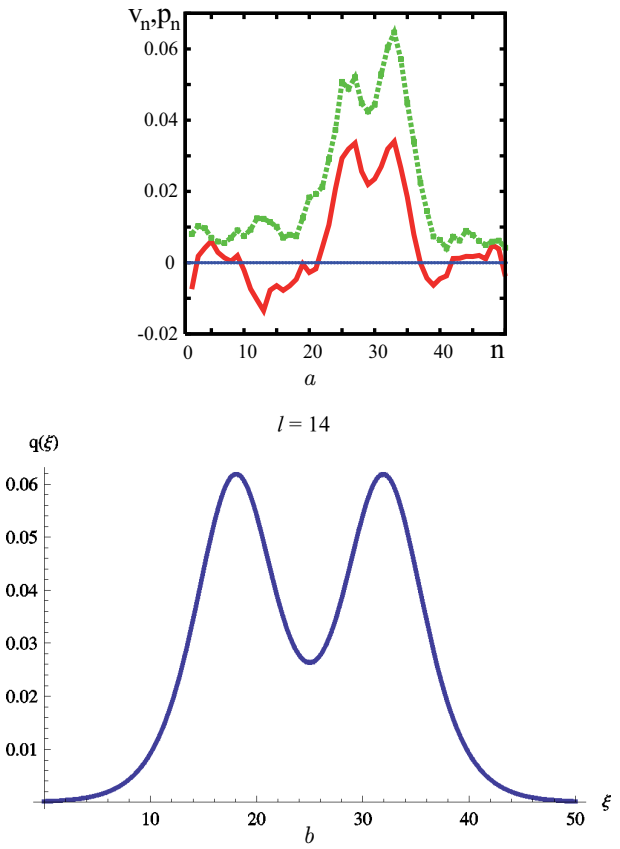

Fig. 4. Results of numerical simulations for the electron density (green dashed line) and the velocity distribution (red solid line) at $\bar{U} = 100$ (a). Blue curve corresponds to bisolecttron density profile $q(x)$ is based on the analytical results (64) at $l = l_0 = 14$ (b)

can be approximated near the minimum with high degree of precision by the anharmonic potential U_c (see Eq. (25)) (for more details, see [30]).

The parameter values used in the simulations were: $\eta = 2.5a, J_0 = 0.02$ ($2D$), $\tau = J_0/(\hbar\,\Omega_{\rm Morse}) = 20$, for three different values of the Hubbard parameter $\bar{U} = U/\hbar\Omega_{\rm Morse}$, namely $\bar{U} = 20, 60, 70, 100$, the lowest of which, $\bar{U} = 20$, for the parameters of alpha-proteins corresponds to $U = 0.004$–0.02 eV, and the upper value $\bar{U} = 100$, respectively, corresponds to $U = 0.02$–0.1 eV.

The results of numerical simulations for the electron density and the velocity distribution of solectron pairs with Hubbard repulsion on the Morse lattice are shown of Figs. 2–5 (a). In Figs. 2–5 (b), we show the charge density function within our analytical model for various values of the Coulomb repulsion, which determines the distance between the maxima of the one-electron functions. We define the charge density function in elementary charge units in a usual way as $q(\xi) = \Phi_1^2(\xi) + \Phi_1^2(\xi)$, where $\Phi_i(\xi)$ are functions determined by expressions (64), and $l = l_0$ as given by relation (70).

Although the numerical and analytical results are obtained in slightly different models of the anharmonic lattice and the Coulomb repulsion, there is a good qualitative agreement in both approaches. In particular, we see that electrons are localized in the bisolectron state, the profile of which depends on the strength of the Coulomb repulsion with the tendency to the splitting of one maximum into two maxima, as the Coulomb repulsion increases.

Notice that the parameter values used in the numerical simulations correspond to a relatively high

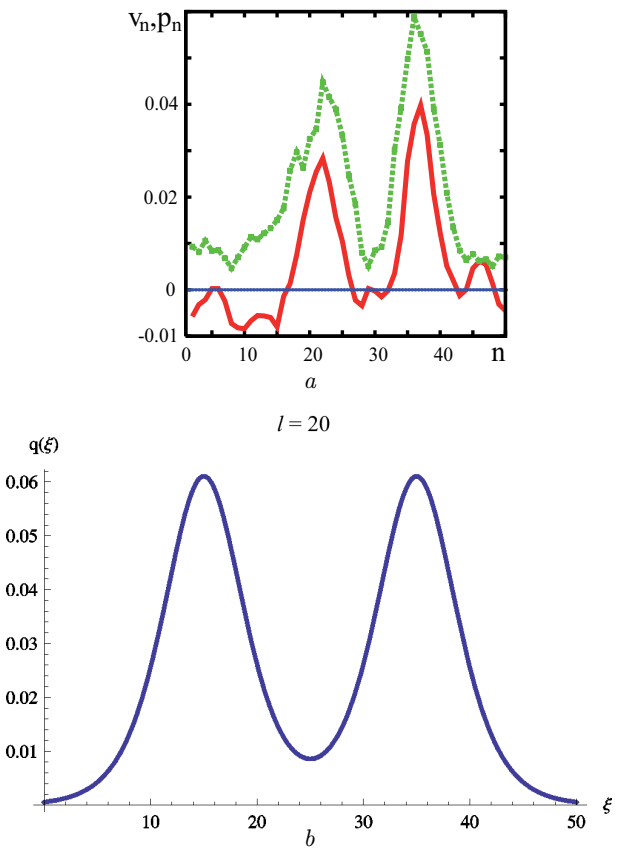

Fig. 5. Results of numerical simulations for the electron density (green dashed line) and the velocity distribution (red solid line) at $\bar{U} = 100$ (a). Blue curve corresponds to bisolecttron density profile $q(x)$ is based on the analytical results (64) at $l = l_0 = 20$ (b)

non-adiabaticity of the system and a strong anharmonicity. Nevertheless, the comparison of the figures corresponding to four different values of the Hubbard term in numerical simulations and, respectively, the Coulomb term in the analytical model shows that our analytical model gives rather good results even for quite a strong electron repulsion. In the lowest order of the continuum approximation used in our model, the functions are smooth with one or two maxima depending on the strength of the Coulomb repulsion. The dynamics of the bisolectron and the account of the lattice discreteness manifested in the presence of the Peierls–Nabarro potential [31, 32] will modify the profile of functions and will lead to some radiation of sound waves, which we can see in the results of numerical modeling in Figs. 3–5.

5. Conclusions

We have shown that, in one-dimensional crystal lattices, the anharmonicity of the intersite interactions favors not only the self-trapping of an extra electron, but also the pairing of two electrons with opposite spins in a single lattice soliton deformation well, resulting in the formation of a stable bisolectron state. Such a bisolectron is the bound state of the lattice soliton and two self-trapped electrons in a singlet bisoliton state. This conclusion generalizes the concepts of polaron and bipolaron [1–5] and proves the existence of bisolitons not only in harmonic one-dimensional systems [9–11, 24], but in anharmonic lattices as well. Our analytical model explains the results of numerical simulations for lattices with anharmonic Morse potential describing the intersite interactions, with two extra electrons in it [25–28]. We have found explicitly the expressions for the lattice deformation and the two-electron wave functions for lattices with cubic and quartic anharmonicities. We have also calculated the energies of the bisolectrons for these two types of anharmonicities and shown that the bisolectrons can move with velocities up to the velocity of sound in the lattice, and the corresponding energy and momentum are finite in the whole interval of bisolectron velocities.

We have studied the role of the Coulomb repulsion in the formation of bisolectrons in anharmonic lattices. We have shown that, with account of the Coulomb repulsion between the electrons, their envelope function in a bisolectron state can have one or two maxima, the distance between which is determined by the balance of the gain of energy due to the binding to the lattice deformation and the loss of energy due to the Coulomb repulsion. The results of the analytical study of two electrons in a lattice with cubic anharmonicity with account of their Coulomb repulsion are in good agreement with the numerical simulations of two electrons in an anharmonic Morse lattice with account of the Hubbard electron-electron repulsion in a broad range of parameter values.

The results obtained here are valid for systems, whose parameter values satisfy the adiabaticity conditions, i.e., for systems with intermediate values of the electron-lattice coupling and the not too large nonadiabaticity parameter (the ratio between characteristic phonon energy and electron band

width). This is a large class of low-dimensional compounds, including biological macromolecules (DNA and α-helical polypeptides) [6, 8, 23, 33], polydiacetylene [34–36], conducting platinum chains and conducting polymers [37], salts of transition metals (PbSe, PbTe, PbS) [38–41], superconducting cuprates [42–46], *etc*. These compounds find numerous applications in microelectronics and nanotechnologies or play the important role in living systems. This explains our interest in studying the nonlinear effects in such systems. In the following papers, we will study a possibility of the pairing of two electrons in a triplet state in anharmonic lattices.

This research was supported by the Spanish Ministerio de Ciencia e Innovacion under grant MAT2011-26221. L. Brizhik acknowledges the partial support from the Fundamental Research Grant of the National Academy of Sciences of Ukraine.

1. L.D. Landau, Phys. Z. Sowjetunion. **3**, 664 (1933).
2. S.I. Pekar, *Untersuchungen über die Elektronentheorie* (Akademie, Berlin, 1954).
3. E.I. Rashba, Izv. Akad. Nauk USSR, Ser. Fiz. **21**, 37 (1957).
4. A.S. Alexandrov and N. Mott, *Polarons and Bipolarons* (World Scientific, Singapore, 1995).
5. *Polarons in Advanced Materials*, edited by A.S. Alexandrov (Springer, Berlin, 2007).
6. A.S. Davydov, *Solitons in Molecular Systems* (Reidel, Dordrecht, 1991).
7. *Davydov's Soliton Revisited. Self-Trapping of Vibrational Energy in Proteins*, edited by A.L. Christiansen and A.C. Scott (Plenum Press, New York, 1983).
8. A.C. Scott, Phys. Rep. **217**, 1 (1992).
9. L.S. Brizhik and A.S. Davydov, J. Low Temp. Phys. **10**, 748 (1984).
10. L.S. Brizhik and A.S. Davydov, J. Low Temp. Phys. **10**, 748 (1984).
11. L.S. Brizhik, J. Low Temp. Phys. **12**, 437 (1986).
12. A.S. Davydov and A.V. Zolotaryuk, Phys. Stat. Sol. (b) **115**, 115 (1983).
13. A.S. Davydov and A.V. Zolotaryuk, Phys. Lett. A **94**, 49 (1983).
14. A. S. Davydov and A. V. Zolotaryuk, Phys. Scripta **30**, 426 (1984).
15. M.G. Velarde, L Brizhik, A.P. Chetverikov, L. Cruzeiro, V. Ebeling, and G. Rö pke, Int. J. Quant. Chem. **112**, 551 (2012).
16. M.G. Velarde, L. Brizhik, A.P. Chetverikov, L. Cruzeiro, V. Ebeling, and G. Röpke, Int. J. Quant. Chem. **112**, 2591 (2012).
17. M. Toda, *Theory of Nonlinear Lattices* (Springer, New York, 1989).
18. M. Toda, *Nonlinear Waves and Solitons* (KTK Sci. Publ., Tokyo, 1989).
19. D.J. Korteweg and G. de Vries, Phil. Mag. **39**, 442 (1895).
20. C.I. Christov, G.A. Maugin, and M.G. Velarde, Phys. Rev. E **54**, 3621 (1996).
21. M. Remoissenet, *Waves Called Solitons* (Springer, Berlin, 1999).
22. V.I. Nekorkin and M. G. Velarde, *Synergetic Phenomena in Active Lattices. Patterns, Waves, Solitons, Chaos* (Springer, Berlin, 2002).
23. T. Dauxois and M. Peyrard, *Physics of Solitons* (Cambridge Univ. Press, Cambridge, 2006).
24. L. Cruzeiro, J.C. Eilbeck, J.L. Marin, and F.M. Russell, Eur. Phys. J. B **42**, 95 (2004).
25. M.G. Velarde, Ch. Neissner, Int. J. Bifurcation Chaos, **18**, 885 (2008).
26. M.G. Velarde, W. Ebeling, A.P. Chetverikov, Int. J. Bifurcation Chaos **18**, 3815 (2008).
27. D. Hennig, M.G. Velarde, W. Ebeling, and A.P. Chetverikov, Phys. Rev. E **78**, 066606 (2008).
28. M.G. Velarde, J. Comput. Appl. Math. **233**, 1432 (2010).
29. W. Ebeling, M.G. Velarde, and A.P. Chetverikov, Cond. Matt. Phys. **12**, 633 (2009).
30. L. Brizhik, A.P. Chetverikov, W. Ebeling, G. Rö pke, and M. G. Velarde, Phys. Rev. B 85, 245105 (2012).
31. L. Brizhik, L. Cruzeiro-Hansson, A. Eremko, and Yu. Olkhovska, Phys. Rev. B **61**, 1129 (2000).
32. L. Brizhik, L. Cruzeiro-Hansson, A. Eremko, and Yu. Olkhovska, Synth. Met. **109**, 113 (2000).
33. V.D. Lakhno and V.B. Sultanov, J. Appl. Phys. **112**, 064701 (2012).
34. E.G. Wilson, J. Phys. C **16** 6739 (1983).
35. K.J. Donovan and E.G. Wilson, Phil. Mag. B **44**, 9 (1981).
36. A.A. Gogolin, Pis'ma Zh. Eksp. Teor. Phys. **43**, 395 (1986)
37. *Electronic Properties of Inorganic Quasi-One-Dimensional Compounds*, edited by P. Monceau, Part II, (Reidel, Dordrecht, 1985).
38. B.G. Streetman and B. Sanjay, *Solid State Electronic Devices* (Prentice-Hall, Englewood Cliff, NJ, 2000).
39. Y. Zhang, X. Ke, C. Chen, and P.C. Kent, Phys. Rev. B **80**, 024303 (2009).
40. *Lead Selenide (PbSe) Crystal Structure, Lattice Parameters, Thermal Expansion*, edited by O. Madelung, U. Rössler, and M. Schultz (Springer, Berlin, 2005), Vol. 41C, available at: http://www.springermaterials.com.
41. J. Androulakis, Y. Lee, I. Todorov *et al.*, Phys. Rev. B **83**, 195209 (2011).
42. C. Falter and G.A. Hoffmann, Phys. Rev. B **64**, 054516 (2001).
43. K.-P. Bohnen, R. Heid, and M. Krauss, Europhys. Lett. **64**, 104 (2003).
44. R.J. McQueeney, Y. Petrov, T. Egami *et al.*, Phys. Rev. Lett. **82**, 628 (1999).

45. T.P. Devereaux, T. Cuk, Z.-X. Shen, and N. Nagaosa, Phys. Rev. Lett. **93**, 117004 (2004)
46. J.-H. Chung, T. Egami, R.J. McQueeney *et al.*, Phys. Rev. B **67**, 014517 (2003).

Received 29.03.13

Л. Брижик, О.П. Четверіков,
В. Ебелінг, Г. Ръопке, М.Г. Веларде

СТАБІЛІЗУЮЧА РОЛЬ АНГАРМОНІЗМУ ҐРАТКИ У ДИНАМІЦІ БІСОЛІТОНІВ

Р е з ю м е

В роботі показано можливість зв'язування двох електронів або дірок у локалізованому бісолітонному стані, який називається також бісолектроном, завдяки взаємодії з локальною деформацією ангармонічного ланцюжка, яка може перевищувати кулонівське відштовхування між зарядами. Показано, що бісолітони є динамічно стійкими також при швидкості, рівній швидкості звуку у ланцюжку, а їх енергія та момент кількості руху мають скінченне значення в усьому інтервалі швидкостей аж до швидкості звуку. Розраховано енергію зв'язування та критичне значення кулонівського відштовхування, при якому бісолітон розпадається на два вільні електросолітони. Оцінено значення цих величин для параметрів, що типові для макромолекул і деяких електропровідних одновимірних систем та показано, що кулонівське відштовхування в них є достатньо слабким порівняно з енергією зв'язування. Результати нашої аналітичної моделі добре пояснюють результати чисельного моделювання в широкому інтервалі параметрів задачі.