ELECTRON SELF-TRAPPING IN ANISOTROPIC TWO-DIMENSIONAL LATTICES: 1. NUMERICAL SIMULATION

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Self-trapped (spontaneously localized) electron states are numerically investigated in a discrete anisotropic two-dimensional electron-phonon lattice. Such a lattice is used as a model of low-dimensional compounds, in the range of parameters characteristic of materials of the conjugated polymers (polydiacetylenes), for which the account is taken of the interchain interactions. The parametric plot is obtained, which shows the range of numerical values of the intrachain and interchain parameters, for which the ground state of an extra electron (hole or exciton) corresponds to a self-trapped soliton-like extended state, to a localized 'small polaron' state, or to a fully delocalized state.

Introduction

In this paper, we investigate numerically the possibility of the existence, within a certain range of the parameters, of self-trapped (or so-called spontaneously localized) electron states in a discrete isotropic and anisotropic two-dimensional molecular lattice with one extra quasiparticle in it (electron, hole, or exciton). For simplicity we refer to this quasiparticle as an electron. The analytic analysis of the results obtained here, will be given in the second part of the paper.

It is known that the electron-phonon coupling can result in some very specific features which are particularly important in low-dimensional systems. However, the general exact solution of the electron-phonon problem is not known even in the simplest $1D$ case. Thus, this problem is considered either for very small molecular clusters or within some approximation based on a perturbation scheme. There are three possibilities for the choice of such a "perturbation": either the electron-phonon interaction is treated (*i*) in the weak coupling or (*ii*) strong coupling limits, resulting in the formation of an almost free electron or small polaron ground states, respectively, or (*iii*) the adiabatic approximation is assumed which is valid provided that the kinetic energy of the lattice is large when compared with that of a relatively light electron which forms a large polaron.

In the case of a $1D$ system, the moderately strong electron-phonon coupling with acoustical phonons leads to the self-trapping of extra electrons and formation of the Davydov soliton, which has been intensively studied both numerically and analytically (see, e.g., [1, 2]). The corresponding system of one-dimensional equations can be reduced, in the continuum limit for the description of excitations in the form of travelling waves with small velocities of propagation, to the nonlinear Shrödinger equation (NLSE) [1] with an attractive cubic nonlinearity term. Its exact soliton solution is well-known. The idea of quasiparticle localization due to the electron-phonon coupling has turned out to be useful in providing an explanation of some special properties of low-dimensional systems (polypeptides, organic and inorganic low-dimensional conducting materials, etc.) in the range of the intermediate values of the electron-phonon coupling when neither the 'small polaron' nor 'weak coupling' (almost free electron) approximation is valid [3]. The stability of a one-dimensional molecular soliton in interaction with external perturbations, including sound waves, electromagnetic fields, chain inhomogeneities, etc., has been proved both numerically and analytically. Another aspect of this problem, connected with the properties of solitons in more complex systems, like alpha-helix or the system of parallel chains with a nonzero interchain exchange interaction, has been studied in [4 – 9] and [10], respectively.

At the same time, however, little is known about the possibility of the existence of spontaneously localized electron-phonon states and their properties, if they exist, in higher dimensions, in spite of numerous investigations of $2D$ and $3D$ solitons in other physical systems (e.g., magnetized plasma, arrays of optical fibres, etc.). This problem is of special importance

not only for almost isotropic $2D$ compounds, but also for strongly anisotropic quasi-$1D$ systems since such systems always possess some nonzero interchain interactions. In particular, the possibility of electron localization in an isotropic $2D$ lattice has been shown numerically in [11, 12] within some approximation, and a $2D$ nonlinear Holstein model has been studied in [13].

1. Hamiltonian of the System and Dynamic Equations

We consider a square discrete molecular lattice (anisotropic in the general case) with an extra electron and, for simplicity, take into account only the interaction between the nearest neighbours. If the values of the physical parameters in one direction, say, 'x'-direction, are much bigger than those in the other one, say, 'y'-direction, such a lattice can be referred to as a system of parallel chains, or as an isotropic $2D$ lattice in the other limiting case of equal values of parameters in both directions.

Such a system can be described in the general case by the Fröhlich Hamiltonian which is a sum of the Hamiltonians describing electron, phonons, and electron-phonons interactions:

$$\hat{H} = \hat{H}_e + \hat{H}_{\rm ph} + \hat{H}_{\rm int}, \tag{1}$$

which have the following form in the site representation:

$$\hat{H}_e = \sum_{n,m} \Big[\mathcal{E}_0 A^+_{n,m} A_{n,m} -$$

$$-J_x (A^+_{n,m} A_{n+1,m} + A^+_{n+1,m} A_{n,m}) -$$

$$-J_y (A^+_{n,m} A_{n,m+1} + A^+_{n,m+1} A_{n,m})\Big], \tag{2}$$

$$\hat{H}_{\rm ph} = \frac{1}{2} \sum_{n,m} \Big(\frac{\hat{P}^2_{n,m}}{M} + \frac{\hat{Q}^2_{n,m}}{M} + K_x [(\hat{U}_{n,m} - \hat{U}_{n+1,m})^2 + (\hat{V}_{n,m} - \hat{V}_{n+1,m})^2] +$$

$$+ K_y [(\hat{U}_{n,m} - \hat{U}_{n,m+1})^2 + (\hat{V}_{n,m} - \hat{V}_{n,m+1})^2] \Big), \tag{3}$$

$$\hat{H}_{\rm int} = \sum_{n,m} A^+_{n,m} A_{n,m} \big[\chi_x (\hat{U}_{n+1,m} - \hat{U}_{n-1,m}) +$$

$$+ \chi_y (\hat{V}_{n,m+1} - \hat{V}_{n,m-1})\big]. \tag{4}$$

Here, $A^+_{n,m}$ ($A_{n,m}$) are the creation (annihilation) operators of an electron at the site (n,m) and $\hat{U}_{n,m}$, $\hat{V}_{n,m}$ and $\hat{P}_{n,m}$, $\hat{Q}_{n,m}$ are, respectively, the longitudinal and transverse components of the vector operator of molecule displacements and their conjugated momenta, $\mathcal{E}_0 - 2J_x - 2J_y$ is the electron energy band bottom, J_x, J_y are the exchange interaction energies, and χ_x, χ_y are the electron-phonon coupling constants in, respectively, the x and y directions, and K_x, K_y are the corresponding elasticity coefficients.

We assume the validity of the adiabatic approximation [1] and take the ground state of the system in the form

$$|\Psi\rangle = \sum_{n,m} \varphi_{n,m} \exp\{-\hat{\sigma}\} A^+_{n,m} |0\rangle, \tag{5}$$

which satisfies the normalization condition

$$\langle \Psi | \Psi \rangle = 1 \tag{6}$$

with $\hat{\sigma} = \frac{1}{i\sqrt{\hbar}} \sum_{n,m} \Big[U_{n,m}(t) \hat{P}_{n,m} + V_{n,m}(t) \hat{Q}_{n,m} -$

$$- P_{n,m}(t) \hat{U}_{n,m} - Q_{n,m} \hat{V}_{n,m}\Big]. \tag{7}$$

Here, $U_{n,m}, P_{n,m}, (V_{n,m}, Q_{n,m})$ are the average values of molecule displacements and canonically conjugated momenta in state (5) in the x (y) direction, $\varphi_{n,m}$ is the probability amplitude of the electron being at the (n,m) site which satisfies the normalization condition

$$\sum_{n,m} |\varphi_{n,m}|^2 = 1. \tag{8}$$

In a $1D$ case, this condition is, to a certain extent, less important for one extra electron, as Eq.(8) determines the amplitude of a soliton via its width and vice versa. However, this condition becomes essential in the many-electron problems as, effectively, it takes into account the quantum statistics of quasiparticles. And, as will be shown below, this condition leads to some nontrivial effects in a $2D$ lattice even in the case of just one extra electron.

In a standard way, we can obtain the energy functional $\mathcal{H} = \langle \Psi | \hat{H} | \Psi \rangle$ as

$$\mathcal{H} = \sum_{n,m} \Big((\mathcal{E}_0 + \mathcal{W}) |\varphi_{n,m}|^2 -$$

$$- J_x \varphi^*_{n,m} (\varphi_{n+1,m} + \varphi_{n-1,m}) -$$

$$- J_y \varphi^*_{n,m} (\varphi_{n,m+1} + \varphi_{n,m-1}) +$$

$$+ |\varphi_{n,m}|^2 \big[b\chi_x (U_{n+1,m} - U_{n-1,m}) +$$

$$+ a\chi_y\,(V_{n,m+1}\,-\,V_{n,m-1})]\Big) \qquad (9)$$

where

$$\mathcal{W} = \frac{1}{2}\sum_{n,m}\Big(\frac{P^2_{n,m}}{M}\,+\,\frac{Q^2_{n,m}}{M}\,+$$

$$+K_x[(U_{n,m}-U_{n+1,m})^2+(V_{n,m}-V_{n+1,m})^2]+$$

$$+K_y[(U_{n,m}-U_{n,m+1})^2+(V_{n,m}-V_{n,m+1})^2]\Big) \qquad (10)$$

is the energy of lattice deformation.

We determine the variational variables $\varphi_{n,m}$ and $U_{n,m}$, $V_{n,m}$ from the extremum condition of $\mathcal{H}$ (9). The corresponding system of equations reads

$$P_{n,m}\,=\,M\frac{dU_{n,m}}{dt}, Q_{n,m}\,=\,M\frac{dV_{n,m}}{dt}. \qquad (11)$$

$$i\,\hbar\frac{d\varphi_{n,m}}{dt}\,=\,(\mathcal{E}_0\,+\mathcal{W}\,)\,\varphi_{n,m}\,-$$

$$-\,J_x\,(\varphi_{n+1,m}\,+\,\varphi_{n-1,m})-$$

$$-\,J_y\,(\varphi_{n,m+1}\,+\,\varphi_{n,m-1})+$$

$$+\,\big[\chi_x\,b\,(U_{n+1,m}\,-\,U_{n-1,m})+$$

$$+\chi_y a\,(V_{n,m+1}\,-\,V_{n,m-1})\big]\varphi_{n,m}, \qquad (12)$$

$$M\frac{d^2U_{n,m}}{dt^2}\,=\,-K_x\,(2\,U_{n,m}\,-\,U_{n+1,m}\,-U_{n-1,m})-$$

$$-K_y\,(2\,U_{n,m}\,-\,U_{n,m+1}\,-U_{n,m-1})+$$

$$+\,b\,\chi_x\,(|\varphi_{n+1,m}|^2\,-\,|\varphi_{n-1,m}|^2), \qquad (13)$$

$$M\frac{d^2V_{n,m}}{dt^2}\,=\,-K_x\,(2\,V_{n,m}\,-\,V_{n+1,m}\,-V_{n-1,m})-$$

$$-K_y\,(2\,V_{n,m}\,-\,V_{n,m+1}\,-V_{n,m-1})+$$

$$+\,a\,\chi_y\,(|\varphi_{n,m+1}|^2\,-\,|\varphi_{n,m-1}|^2). \qquad (14)$$

These equations have, at least, two constants of motion, one of which is equivalent to the total electron probability, which satisfies the normalization condition (8), and the second one is the total energy (9). Notice that, in the case of an isolated molecular chain, *i.e.*, when all parameters in the y-direction are equal to zero, the system of equations (12)-(14) reduces to the Davydov system of equations [1] which admits a localized bound electron-phonon solution in the form of a molecular soliton.

It is useful to introduce dimensionless units

$$Y\,=\,\frac{C_y}{E_s},\quad k_x\,=\,\frac{K_x\,\hbar^2}{M\,J_x^2},\quad k_y\,=\,\frac{K_y\,\hbar^2}{M\,J_x^2},$$

$$j_y\,=\,\frac{J_y}{J_x},\quad E_s\,=\,\frac{b^2 M\,J_x}{\hbar^2},\quad E_0\,=\,\frac{\mathcal{E}_\prime}{J_x},$$

$$C_x\,=\,\frac{\chi_x\,b^2}{J_x},\quad C_y\,=\,\frac{\chi_y\,a\,b}{J_x},\quad X\,=\,\frac{C_x}{E_s},$$

$$\tau\,=\,\frac{J_x t}{\hbar},\quad u\,=\,\frac{U}{b},\quad v\,=\,\frac{V}{b}, \qquad (15)$$

in which Eqs. (12)-(14) take the following form:

$$i\,\frac{d\varphi_{n,m}}{d\tau}\,=\,(E_0\,+W\,)\,\varphi_{n,m}\,-$$

$$-\,(\varphi_{n+1,m}\,+\,\varphi_{n-1,m})\,-\,j_y\,(\varphi_{n,m+1}\,+\,\varphi_{n,m-1})+$$

$$+\,\big[C_x\,(u_{n+1,m}\,-\,u_{n-1,m})+$$

$$+\,C_y\,(v_{n,m+1}\,-\,v_{n,m-1})\big]\,\varphi_{n,m}, \qquad (16)$$

$$\frac{d^2u_{n,m}}{d\tau^2}\,=\,-k_x\,(2\,u_{n,m}\,-\,u_{n+1,m}\,-u_{n-1,m})-$$

$$-k_y\,(2\,u_{n,m}\,-\,u_{n,m+1}\,-u_{n,m-1})+$$

$$+\,X\,(|\varphi_{n+1,m}|^2\,-\,|\varphi_{n-1,m}|^2), \qquad (17)$$

$$\frac{d^2v_{n,m}}{d\tau^2}\,=\,-k_x\,(2\,v_{n,m}\,-\,v_{n+1,m}\,-v_{n-1,m})-$$

$$-k_y\,(2\,v_{n,m}\,-\,v_{n,m+1}\,-v_{n,m-1})+$$

$$+\,Y\,(|\varphi_{n,m+1}|^2\,-\,|\varphi_{n,m-1}|^2). \qquad (18)$$

Here,

$$H\,=\,\sum_{n,m}\Big((E_0\,+\,W)\,|\varphi_{n,m}|^2\,-$$

$$-\,\varphi^*_{n,m}(\varphi_{n+1,m}+\varphi_{n-1,m})-$$

$$-j_y\,\varphi^*_{n,m}(\varphi_{n,m+1}+\varphi_{n,m-1})+$$

$$+|\varphi_{n,m}|^2\big[C_x\,(u_{n+1,m}\,-\,u_{n-1,m})\,+$$

$$+\,C_y\,(v_{n,m+1}\,-\,v_{n,m-1})\big]\Big), \qquad (19)$$

$$W\,=\,\frac{1}{2}\,E_s\,\sum_{n,m}\Big(p^2_{n,m}+q^2_{n,m}\,+$$

$$+\,k_x[(u_{n,m}-u_{n+1,m})^2+(v_{n,m}-v_{n+1,m})^2]+$$

$$+ k_y[(u_{n,m} - u_{n,m+1})^2 + (v_{n,m} - v_{n,m+1})^2]\Big), \quad (20)$$

and

$$p_{n,m} = \frac{du_{n,m}}{d\tau}, \quad q_{n,m} = \frac{dv_{n,m}}{d\tau}. \quad (21)$$

For slowly varying functions, we can pass to the continuum approximation and rewrite the system of equations (16)-(18), keeping only the second spatial derivatives, as

$$\left[i\frac{\partial}{\partial\tau} - \lambda + \frac{\partial^2}{\partial x^2} + j_y\frac{\partial^2}{\partial y^2} - \right.$$

$$\left. - \left(2C_x\frac{\partial u}{\partial x} + 2C_y\frac{\partial v}{\partial y}\right)\right]\varphi(x,y) = 0, \quad (22)$$

$$\left(\frac{\partial^2}{\partial\tau^2} - k_x\frac{\partial^2}{\partial x^2} - k_y\frac{\partial^2}{\partial y^2}\right)u(x,y) =$$

$$= 2X\frac{\partial|\varphi(x,y)|^2}{\partial x}, \quad (23)$$

$$\left(\frac{\partial^2}{\partial\tau^2} - k_x\frac{\partial^2}{\partial x^2} - k_y\frac{\partial^2}{\partial y^2}\right)v(x,y) =$$

$$= 2Y\frac{\partial|\varphi(x,y)|^2}{\partial y}, \quad (24)$$

where $\lambda = (E_0 + W - 2 - 2j_y)$.

In the isotropic case, we find from the last two equations

$$\left\{\frac{\partial^2}{\partial\tau^2} - k\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]\right\}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) =$$

$$= 2X\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)|\varphi(x,y)|^2, \quad (25)$$

and, hence, in the adiabatic approximation

$$\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) = -\frac{2X}{k}|\varphi|^2. \quad (26)$$

Substituting now (26) into (22), we get $2D$ isotropic NLSE with an attractive potential:

$$i\frac{\partial\varphi(x,y)}{\partial\tau} = \lambda\varphi(x,y) - \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\varphi(x,y) -$$

$$-2g|\varphi(x,y)|^2\varphi(x,y), \quad (27)$$

where g is the nonlinearity parameter:

$$g = \frac{2CX}{k} = \frac{2\chi_x^2 b^2}{J_x K_x}. \quad (28)$$

It is known that solitons of the continuous $2D$ NLSE are unstable with respect to the collapse [14 – 17]. Therefore, the question does arise as to whether molecular solitons are relevant to and stable in real systems. Let us note, however, that both the simplified continuous and even discrete $2D$ NLSEs are unlikely to be good approximations to the description of properties of strongly localized excitations. Moreover, the above objections are not relevant when we consider real discrete lattices: when the size of a soliton decreases so that its width becomes comparable with the lattice spacing, the continuum approximation is not valid, at least not within the accuracy of the second space derivatives of the wavefunction, *i.e.*, higher order derivatives should be included in the NLSE. Their inclusion increases the dispersion of the wavepacket and, under certain conditions, can stabilize the soliton [18 – 20]. The exact solution is not known even for the continuum $2D$ NLSE with higher order derivatives. Therefore, the most straightforward way to study this problem is to investigate it numerically and, in the next section, we present results of such an investigation.

2. Description of a Numerical Model

We have performed numerical simulations of the system of equations (16)-(18) on a square grid of 101×101 sites with fixed boundary conditions which are equivalent to the elastic reflection of waves from the boundaries. As will be shown below, this scattering has little influence on the localized electron states. Our calculations show that a localized state, when it exists, is stable with respect to the interaction with both sound waves and electron radiation fields which are reflected from the boundaries. This behaviour changes dramatically when the size of the localization spreads out and covers a large part of the grid. To study this, we took the initial electron wavefunction in the form of an anisotropic Gaussian wave packet, normalized to unity, which was positioned at the center of the grid and which was spread out over a few lattice sites in both directions. The initial conditions for the deformation fields were chosen to be correlated to the electron field. In this way, we avoided any discontinuities in the calculations and reduced the emission of sound waves caused by the excess of energy of the initial pulse as compared to the energy of the steady-state solution corresponding to the system of dynamical equations (16)-(18).

Our numerical simulations started with the values of the parameters characteristic of the polydiacetylene

(PDA) class of compounds; namely, we fixed lattice spacing $b = 4.9\times10^{-10}$ m and cell mass $M = 1.57\times10^{-25}$ kg, and took the following initial values (see, e.g., [21 – 24]):

$$J_x = 1.05 \times 10^{-19} J, \quad K_x = 69N/m,$$

$$\chi_x = 3.5N/m. \tag{29}$$

Let us recall that an isolated chain with the parameters corresponding to the x-values of the parameters in set (29) is a good adiabatic system in which the ground state of an electron corresponds to the soliton [25]. This was one of the reasons for choosing it in the present investigation. While the numerical values of the intrachain parameters are more or less known [21 – 24, 26], the values of the interchain parameters are much less known besides the fact that they are much smaller than the corresponding intrachain ones and vary in the interval $10^{-1} \div 10^{-3}$ of the corresponding x-values.

Moreover, it has been experimentally observed that the conducting properties and optical spectra of the various compounds with similar structures from this family can be significantly different [27 – 31]. This demonstrates the crucial role of physical parameters: what can seem as an insignificant change of the parameter(s) turns out to lead to a significant change in physical properties. This fact, by itself, suggests a nonlinear nature of the underlying physical mechanisms/processes under certain conditions. And the soliton mechanism discussed here can be one of such possibilities. Indeed, our numerical calculations demonstrate the significant role of physical parameters in the formation and stability of soliton-like structures in $2D$ electron-phonon lattices described by Eqs. (12)-(14).

3. An Important Role of the Second Dimension

Our first experiment involved a numerical simulation with the set of parameters (29) and rather strong interchain interaction parameters, namely: $j_y = 0.1, k_y = 0.1k_x, C_y = C_x/30$. The numerical calculations have shown that the initial wavepacket evolved with time into a peak localized within one lattice site with the maximum value of the probability amplitude, i.e., the height, $A_{\max} = 0.9$.

To investigate the role of the transverse (interchain) interactions, we have then performed a set of simulations for system (16)-(18) with y-values of all parameters changed by the same factor α, i.e., we set $j'_y = \alpha j_y$, $C'_y = \alpha C_y$, $k'_y = \alpha k_y$, where $\alpha = 0.25 \div 8$. If the analogy with $2D$ NLSE were proper, one would expect an ever stronger localization of a quasiparticle with a decrease of the anisotropy of the system, i.e., with $\alpha > 1$. However, on the contrary, it turns out that the region of the electron and deformation localization increases with α. The soliton gets broader and its size covers several lattice sites at $3 < \alpha < 4.5$. At $\alpha > 4.53$, the initial pulse disperses over the whole grid; the larger the α, the quicker the dispersion: at $\alpha = 5$, it takes more than 7000 units of time for the pulse to get delocalized, only 700 at $\alpha = 6$, and the Gaussian packet disperses from the very beginning at $\alpha = 8$. A typical picture of time-dependence of soliton height, within the region of soliton stability $3 < \alpha < 4.5$, is shown in Fig.1.

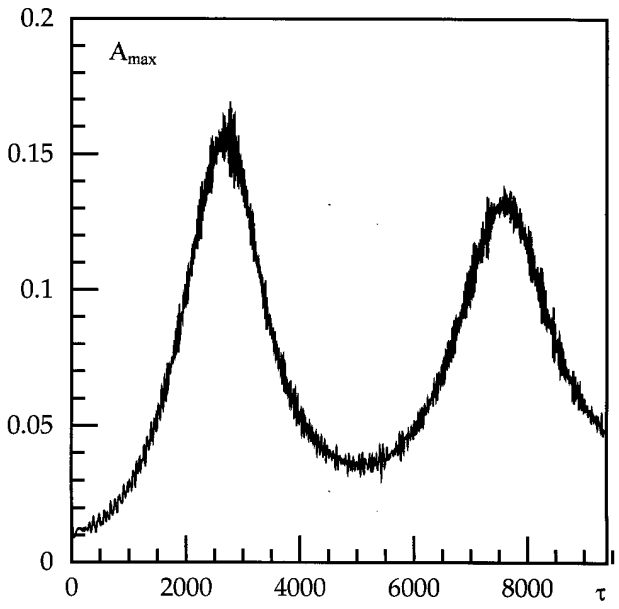
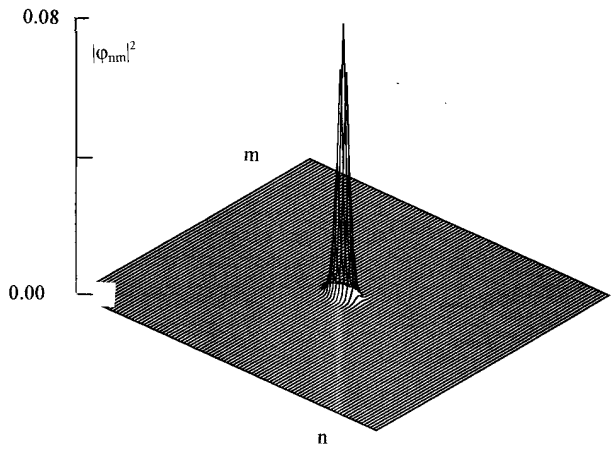


Fig. 1. Time dependence of the soliton height, A_{max}, for $\alpha = 4$

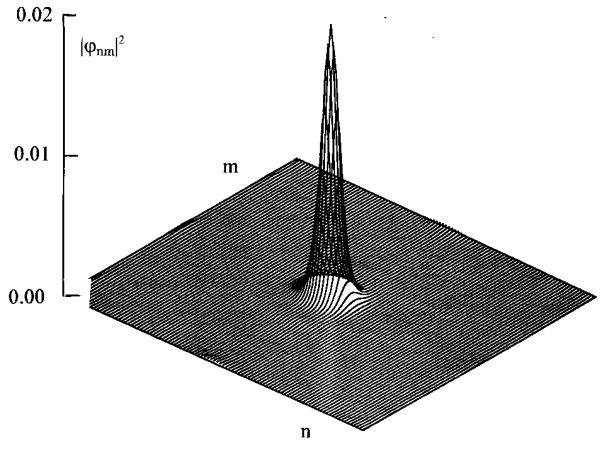
To start with, the initially wide pulse shrinks but, because of the retardation effects in the deformational field, this process overshoots the width value corresponding to the steady-state solution. Later, the soliton shrinks and, when its size becomes too small, begins to spread again. Several such oscillations of the width and, respectively, height (which is connected with the width by the normalization condition (8)), are needed to reach the steady-state solution. The amplitude of these oscillations decreases exponentially with time.

We should also take note of the presence of additional high-frequency oscillations of the soliton height in the steady state. The frequency of these additional



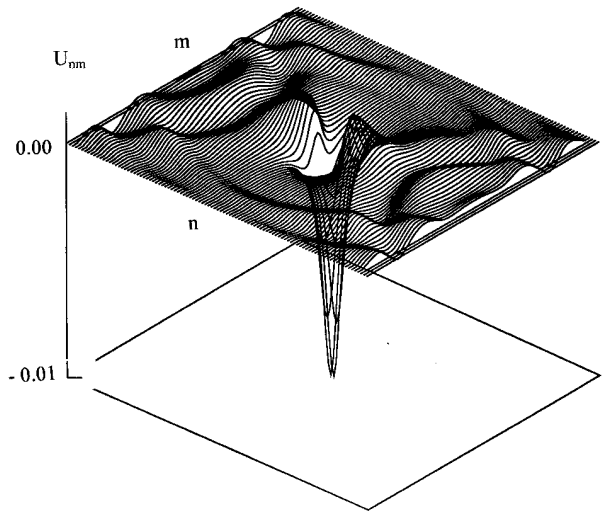
a

Fig. 2,*a*. Electron probability distribution of the initial Gaussian packet for $\alpha = 4.5$ at $\tau = 10$



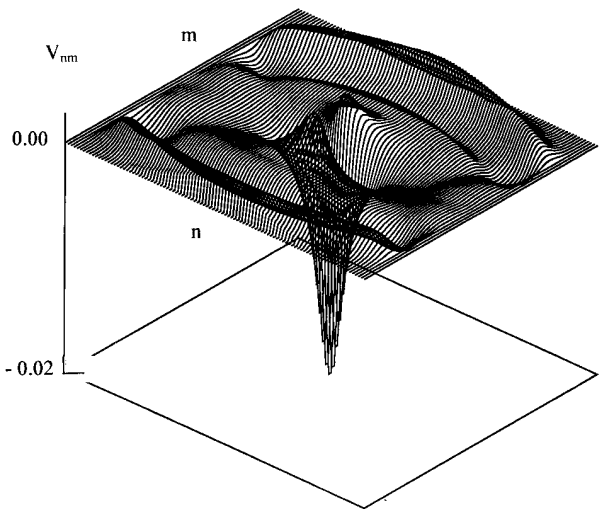
b

Fig. 2,*b*. Electron probability distribution of the initial Gaussian packet for $\alpha = 4.5$ at $\tau = 9500$



a

Fig. 3,*a*. Distribution of the intrachain deformation for $\alpha = 4.5$ at $\tau = 9500$



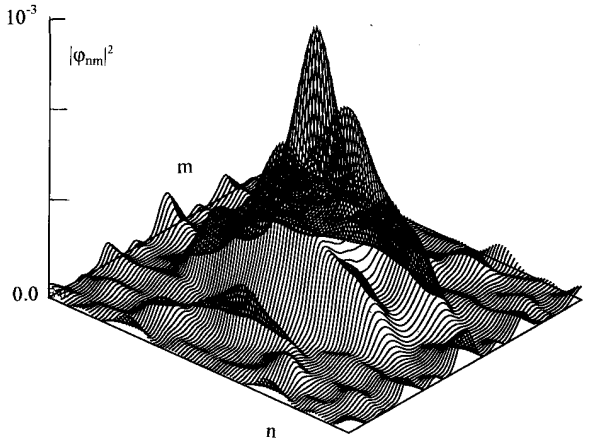
b

Fig. 3,*b*. Distribution of the interchain deformation for $\alpha = 4.5$ at $\tau = 9500$

oscillations depends on the parameters as well, and their amplitude decreases from the value $\delta A = A_{\max} - A_{\min} = 0.15$ at $\alpha = 0.25$ down to $\delta A = 0.01$ at $\alpha = 4.5$. These high-frequency oscillations of the amplitude are connected with lattice discretness and are present in discrete $1D$ chains as well [32].

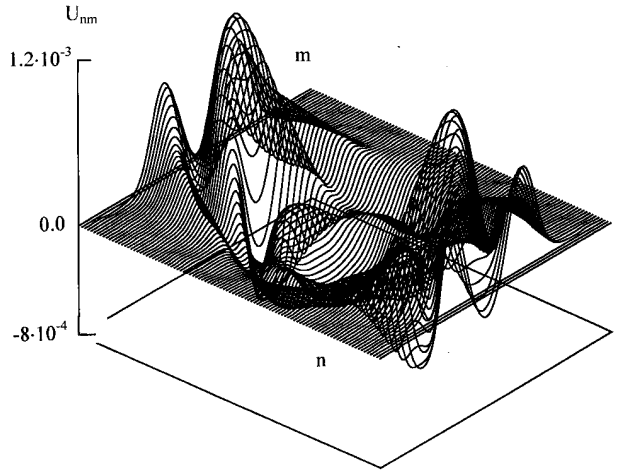
Figs. 2-3 show time evolution of the initial Gaussian packet of the electron probability $\varphi_{n,m}$, intrachain deformation $u_{n,m} - u_{n-1,m}$ and interchain deformation $v_{n,m} - v_{n,m-1}$, respectively, at various times for the values of parameters corresponding to $\alpha = 4.5$.

To understand better the role of each parameter independently, namely, the strength of the interchain exchange interaction, electron-phonon coupling, and elasticity, in the formation of soliton-like structures, we have performed a set of further simulations with one of these three parameters changed and the other two ones fixed starting from the value $\alpha = 4$. Our simulations



a

Fig. 4,*a*. Electron probability distribution of the initial Gaussian packet for $\beta = 0.55$ at $\tau = 5650$



b

Fig. 4,*b*. Distribution of the intrachain deformations for $\beta = 0.55$ at $\tau = 5650$

have shown that a change in k_y causes only small changes in the amplitude and the width of the soliton, as well, as it has only little effect on the time of the soliton formation from the initial Gaussian packet. Much more important are changes of j_y or C_y values. Thus, we set $k_y = 0.4k_x, C_y = C_x/7.5, j_y = \beta$, where the anisotropy parameter of the exchange interaction β varies in the interval $0.1 \div 1.0$. Our simulations have shown that, at $0.1 < \beta < 0.3$, the soliton is anisotropic in shape: it is extremely narrow in the direction perpendicular to chains and extends over three lattice sites along the chain direction. At $\beta = 0.1$, as much as $3/4$ of the electron probability is concentrated within one lattice site and the rest within the two next sites, while the probability is redistributed in the ratio 3:2 at $\beta = 0.3$. Such a narrow soliton is easily pinned by the lattice and/or lattice impurities, and it can move only via some additional mechanisms. Hence, the conducting properties of a system with such values of parameters should have a threshold with respect to the applied voltage and be significantly dependent on the concentration of impurities, temperature, etc.

The width of the soliton in both directions increases with the interchain exchange interaction constant and, in the interval $0.35 < \beta < 0.45$, the electron and deformation distributions correspond to a clean soliton-like configuration. When j_y increases further, the soliton spreads out more and more, the emission of phonons and electron radiation in both directions becomes more intensive and the sound waves and radiation reflected from the boundaries hit the low amplitude broad soliton and destroy it (see Fig. 4).

Our next step involved the investigation of the role of the interchain electron-phonon coupling. We have found that the soliton-like distribution is not affected much by a decrease of C_y by a factor c in the interval [1, 8], since the threshold for the soliton formation can be crossed by a proper choice of other parameters. The time of the soliton formation from an initial Gaussian packet, of course, does depend on the value of C_y. The role of the interchain electron-phonon coupling is crucial and manifests itself more profoundly in the case where the other parameters corresponding to the delocalized electron state. In such a case, the conditions for soliton formation can be satisfied by increasing the value of the interchain electron-phonon coupling. For instance, at $j_y = 0.6$, $k_y = 0.4k_x$, the soliton can be formed if $C_y > C_x/72$. Fig. 5 shows the distribution of the total energy density on a $2D$ lattice with the parameters $j_y = 0.4$, $k_y = 0.4k_x$, $C_y = C_x/7.5$ at the time moment $\tau = 9300$. Clearly, the figure exhibits a localized distribution of energy correlated with the distribution of electron probability and lattice deformations.

To check the role of the initial conditions, we have performed several other simulations started with Gaussian packets of different widths, and have concluded that for this type of packets, the time of soliton formation depends on the width of the initial pulse, provided it is reasonably smooth and extended over several lattice sites.

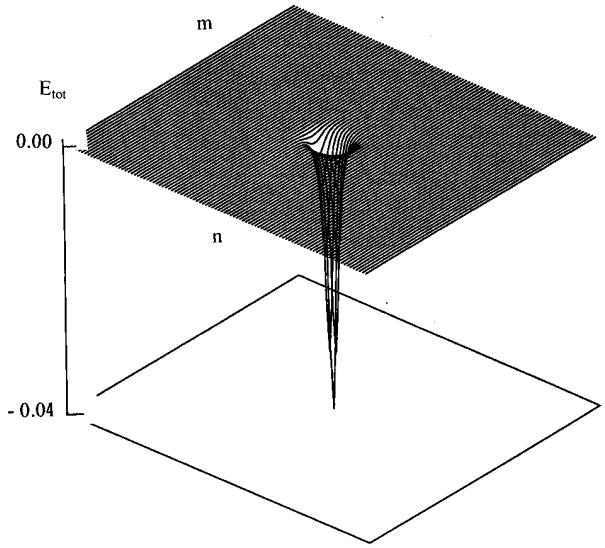


Fig. 5. Distribution of the total energy density$< E_{tot}$, at $j_y = 0.4$, $k_y = 0.4k_x$, $C_y = C_x/7.5$, $\tau = 9300$

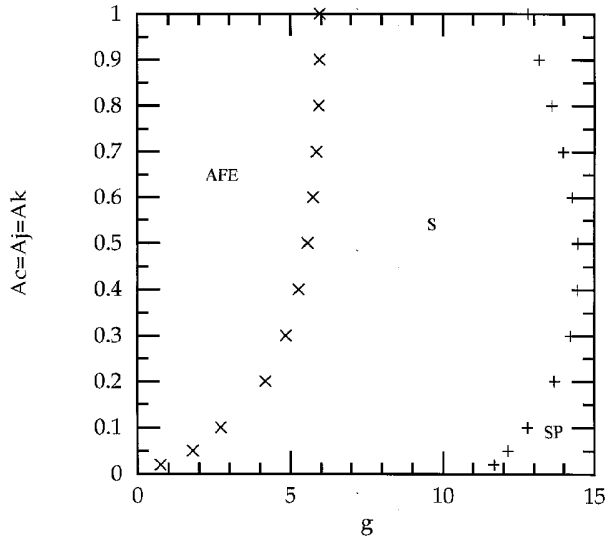


Fig. 6. Parametric diagram of the ground electron states (AFE - almost free electron, S - soliton, SP - small polaron) as a function of nonlinearity g, and anisotropy A

Conclusions

The numerical simulations discussed above are summarized in the form of a parametric diagram shown in Fig. 6 for the case of equal anisotropy of all parameters, $A = J_y/J_x = K_y/K_x = \chi_y/\chi_x$. This diagram shows the ranges of the nonlinearity parameter g determined in (28), in which the ground electron state corresponds to a delocalized, almost free, electron state (AFE), a self-trapped soliton-like state (S) and a strongly localized small polaron state (SP) for the given value of the anisotropy parameter A. Thus, the calculations prove the existence of spontaneously localized bound electron-phonon states, in some range of the values of electron-phonon coupling, exchange interaction energy, and elasticity, both in the cases of the isotropic and anisotropic two-dimensional discrete lattices. The formation of these states has a threshold with respect to these parameters.

Once formed, the localized states are stable with respect to the interaction with sound waves and the electron radiation reflected from the lattice boundaries, which demonstrates the essentially solitonic nature of these states. Note, that a possible role of localized electron states in some systems from the PDA series was discussed in [33 – 35, 30] and the corresponding photoabsorption spectra were explained using this concept. The above conclusion about the threshold character of soliton formation in $2D$ lattices and its dependence on the initial excitation, can explain the experimentally observed [36, 37, 28] dramatic difference in the generation efficiency of the photoabsorption spectra of polycrystalline films of polydiacetylenes for the different laser excitation frequencies. In particular, the generation efficiency using the laser pulses of energy 2.32 eV is more than an order of magnitude lower than at $\hbar\omega = 3.48$ eV. In fact, the results of the present numerical calculation indicate that lower energy pulses are insufficient to excite soliton states and that the initial excitation packets spread all over the lattice with time, have higher energies, and are easily scattered by lattice phonons.

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АВТОЛОКАЛІЗАЦІЯ ЕЛЕКТРОНІВ В АНІЗОТРОПНИХ ДВОВИМІРНИХ КРИСТАЛАХ. 1. ЧИСЕЛЬНЕ МОДЕЛЮВАННЯ

Л. Брижик, Б. П'етт, В.Є. Закржевські

Р е з ю м е

Чисельними методами досліджено автолокалізовані електронні стани в дискретних анізотропних двовимірних кристалах з урахуванням електрон-фононної взаємодії. При відповідних значеннях фізичних параметрів такі системи моделюють квазіодновимірні сполуки класу спряжених полімерів (полідіацетиленів) з урахуванням міжланцюжкової взаємодії. Побудовано параметричні діаграми станів, що визначають області значень параметрів ланцюжків та міжланцюжкової взаємодії, при яких основний стан квазічастинки (електрона, дірки або екситона) відповідає автолокалізованому солітоноподібному стану, полярону малого радіуса або повністю делокалізованому стану.

АВТОЛОКАЛИЗАЦИЯ ЭЛЕКТРОНОВ В АНИЗОТРОПНЫХ ДВУМЕРНЫХ КРИСТАЛЛАХ. 1. ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ

Л. Брижик, Б. Пьетт, В.Е. Закржевски

Р е з ю м е

Численными методами исследованы автолокализированные электронные состояния в дискретных анизотропных двумерных кристаллах с учетом электрон-фононного взаимодействия. При соответствующих значениях физических параметров такие системы молелируют квазиодномерные соединения класса сопряженных полимеров (полидиацетиленов) с учетом межцепочечного взаимодействия. Построены параметрические диаграммы состояний, определяющие области значений параметров внутрицепочечного и межцепочечного взаимодействий, при которых основное состояние квазичастицы (электрона, дырки или экситона) соответствует автолокализированному солитоноподобному состоянию, полярону малого радиуса или полностью делокализированному состоянию.