ELECTRON SELF-TRAPPING IN DISCRETE TWO-DIMENSIONAL LATTICES. II. ANALYTICAL STUDY

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UDC 538.9, 538.915, 517.957

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In the previous paper [1], self-trapped (spontaneously localized) electron states in a discrete, anisotropic, two-dimensional electron-phonon lattice were investigated numerically. Here this problem is studied analytically for an isotropic lattice. It is shown that, in the adiabatic approximation, the continuum limit of the discrete equations leads to a two-dimensional nonlinear Schrödinger equation with an extra term. This extra term comes from the lattice discreteness and is shown to be essential to prevent a soliton from collapsing. This is achieved when the nonlinearity parameter takes values within some finite interval: $g_{c1} < g < g_{c2}$. It is shown, within the variational scheme, that the energy minimum is attained for the delocalized states provided $g < g_{c1}$, and for the strongly localized states (essentially on one lattice site) provided $g > g_{c2}$. The radius of the quasiparticle localization as a function of the electron-phonon coupling constant is evaluated. Some preliminary results on moving solitons are also presented.

Introduction

Studies of electrical and optical properties in low-dimensional materials have revealed the important role of collective excitations and of the electron-phonon coupling which can result in the creation of localized modes. Generally speaking, one-dimensional systems (1DS) have attracted systematic theoretical and experimental studies [2 — 4] which have proved the existence of soliton-like states under certain conditions. At the same time, much less is known about two-dimensional systems (2DS). Some aspects of this problem have been studied for isotropic [5, 6, 8] and anisotropic [1, 7] crystals. In particular, in the first part of this paper [1], the possibility of the existence, within a certain range of parameters, of self-trapped (or so-called spontaneously localized) electron states in a discrete isotropic or anisotropic two-dimensional molecular lattice with one extra quasiparticle (electron, hole, or exciton) has been demonstrated numerically.

Here the possibility of the quasiparticle self-trapping is studied analytically for an isotropic lattice. Using a variational ansatz in the quasimomentum representation, we compute the relation between the width of a soliton and the coupling constant. In particular, we show that this relation admits solutions that correspond to a soliton-like lump when the coupling constant lies within a very specific finite range. When this constant is smaller than the calculated critical value, a localized quasiparticle solution does not exist. We support the validity of our analysis by comparing these predictions with the numerical results obtained previously.

We also show that the system of discrete equations, in the continuum approximation, can be reduced to a two-dimensional nonlinear Schrödinger equation ($2\,D$ NLSE) with extra terms. Although various properties of $2D$ NLSE (continuum and discrete) models in general and $2\,D$ polaron states, in particular, have been studied during the past years and various remarkable phenomena have already been described [10 — 13], some fundamental aspects of soliton states in $2\,D$ structures so far have not been clarified. The extra terms in the $2D$ NLSE, that arise due to the lattice discreteness, are shown to be essential to prevent the soliton collapse. This is shown to be the case when the nonlinearity parameter takes values within a finite interval, namely: $g_{c1} < g < g_{c2}$. This stabilization of the soliton solutions is a result of an interplay between discreteness, dispersion and nonlinearity. We show that, within our variational scheme, the energy minimum is attained for the delocalized states provided $g < g_{c1}$, and for the strongly localized states (to within one lattice site) provided $g > g_{c2}$. Our scheme allows us also to calculate the radius of the quasiparticle localization as a function of the electron-phonon coupling constant.

1. Hamiltonian of the System

Quasiparticle states on a regular $2\,D$ lattice when one takes into account the electron-phonon interaction are described by the Hamiltonian which can be written in

the site representation as

$$\hat{H} = \sum_{\vec{m}} \mathcal{E}_0 A^+_{\vec{m}} A_{\vec{m}} + \sum_{\vec{m},\vec{n}} [-J_{\vec{m},\vec{n}} \left(A^+_{\vec{m}} A_{\vec{n}} + A^+_{\vec{n}} A_{\vec{m}} \right) +$$

$$+\chi_{\vec{m},\vec{n}} A^+_{\vec{m}} A_{\vec{m}} \left(\hat{u}_{\vec{m}} - \hat{u}_{\vec{n}} \right)] + \sum_{\mu,\vec{n}} \frac{\hat{p}^2_\mu(\vec{n})}{2M} +$$

$$+\frac{1}{2} \sum_{\mu,\nu,\vec{n},\vec{m}} w_{\mu,\nu}(\vec{n},\vec{m}) \hat{u}_\mu(\vec{n}) \hat{u}_\nu(\vec{m}). \quad (1)$$

Here $A^+_{\vec{m}}$ ($A_{\vec{m}}$) are the creation (annihilation) operators of the quasiparticle on the site $\vec{m}$ with the corresponding radius-vector coordinate $\vec{R}_{\vec{n}} = \vec{e}_x a_x m + \vec{e}_y a_y n$, $m, n = 0, \pm 1, \pm 2, ...$, $\hat{u}_{\vec{m}}$ and $\hat{p}_{\vec{m}}$ are operators of molecule displacements from their equilibrium positions and the corresponding conjugate momenta, $\mathcal{E}_0$ is the quasiparticle on-site energy, $J_{\vec{m},\vec{n}}$ are the exchange interaction energies, $\chi_{\vec{m},\vec{n}}$ are the electron-phonon coupling constants, $\vec{e}_\mu$ is the unit vector along the μ-axis, $\mu = x, y$, and a_μ is the corresponding lattice spacing, M is the atom mass, and $w_{\mu,\nu}(\vec{n},\vec{m})$ are the lattice elasticity coefficients which are assumed to be constant on the grid: $w_{\mu\mu}(\vec{n}, \vec{n} \pm \vec{e}_x) = w_{\mu\mu}(\vec{n}, \vec{n} \pm \vec{e}_y) = w$.

We study the problem in the adiabatic approximation and choose the vector state of one quasiparticle in the multiplicative form [14] as

$$|\Psi> = \sum_{\vec{n}} \varphi_{\vec{n}} \exp\{-\hat{\sigma}\} A^+_{\vec{n}} |0>, \quad <\Psi|\Psi> = 1 \quad (2)$$

with

$$\hat{\sigma} = \frac{i}{\sqrt{\hbar}} \sum_{\mu,\vec{n}} \left[u_\mu(\vec{n},t) \hat{p}_\mu(\vec{n}) - p_\mu(\vec{n},t) \hat{u}_\mu(\vec{n}) \right]. \quad (3)$$

Here $u_\mu(\vec{n},t)$ and $p_\mu(\vec{n},t)$ are the average values of molecule displacements in the μ direction and of the canonically conjugate momenta in the state (2), $|0>$ is the vacuum state of the quasiparticle and the lattice, $\varphi_{\vec{n}}$ is the probability amplitude of the quasiparticle presence on the $\vec{n}$-th site which satisfies the normalization condition

$$\sum_{n,m} |\varphi_{m,n}|^2 = 1. \quad (4)$$

From Hamiltonian (1), we can obtain, in the adiabatic approximation (2), the energy functional $\mathcal{H} = <\Psi|\hat{H}|\Psi>$, which takes the following form for the isotropic lattice in the nearest neighbour approximation considered here:

$$\mathcal{H} = \sum_{\vec{n}} \{\mathcal{E}_0 \varphi^*_{\vec{n}} \varphi_{\vec{n}} - J[\varphi^*_{\vec{n}} (\varphi_{\vec{n}+\vec{e}_x} + \varphi_{\vec{n}-\vec{e}_x}) -$$

$$-\varphi^*_{\vec{n}} (\varphi_{\vec{n}+\vec{e}_y} + \varphi_{\vec{n}-\vec{e}_y})] + +\varphi^*_{\vec{n}} \varphi_{\vec{n}} \chi \sum_\mu [u_\mu(\vec{n} + \vec{e}_\mu) -$$

$$- u_\mu(\vec{n} - \vec{e}_\mu)]\} + \mathcal{W}. \quad (5)$$

Here $\mathcal{W}$, the phonon energy, is the sum of the kinetic and potential energies

$$\mathcal{W} = \frac{1}{2} \sum_{\vec{n},\mu} \Big\{ \frac{p^2_\mu(\vec{n})}{M} + w_x \left[u_\mu(\vec{n}) - u_\mu(\vec{n} - \vec{e}_x) \right]^2 +$$

$$+w_y \left[u_\mu(\vec{n}) - u_\mu(\vec{n} - \vec{e}_y) \right]^2 \Big\}. \quad (6)$$

2. Variational Analysis

In this section, we perform the variational analysis of the problem. For this, it is convenient to use the quasimomentum representation

$$\vec{k} = k_x \vec{e}_x + k_y \vec{e}_y, \quad k_\mu = \frac{2\pi l_\mu}{Na},$$

$$l_\mu = 0, \pm 1, \pm 2, ...N/2, \quad N_x = N_y = N, \quad (7)$$

using the following transformations:

$$\varphi_{\vec{n}} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} \Phi(\vec{k}) e^{i\vec{k}\vec{n}}, \quad u_\mu(\vec{n}) = \frac{1}{\sqrt{N}} \sum_{\vec{k}} Q_\mu(\vec{k}) e^{i\vec{k}\vec{n}}. \quad (8)$$

The Hamiltonian functional (5) then takes the following form:

$$\mathcal{H} = \sum_{\vec{k}} E(\vec{k}) \Phi^*(\vec{k}) \Phi(\vec{k}) + \frac{1}{2} \sum_{\vec{q},\mu} \left[P^*_\mu(\vec{q}) P_\mu(\vec{q}) + \right.$$

$$\left. + \Omega^2_\mu(\vec{q}) Q^*_\mu(\vec{q}) Q_\mu(\vec{q}) \right] +$$

$$+\frac{1}{\sqrt{N}} \sum_{\vec{k},\vec{q},\mu} S_\mu(\vec{q}) \Phi^*(\vec{k}) \Phi(\vec{k} - \vec{q}) Q_\mu(\vec{q}), \quad (9)$$

where

$$E(\vec{k}) = \mathcal{E}_0 - 2J\cos(k_x a) - 2J\cos(k_y a), \quad (10)$$

$$\Omega^2_\mu(\vec{q}) = \Omega^2(\vec{q}) = \frac{4w}{M} \left(\sin^2 \frac{q_x a}{2} + \sin^2 \frac{q_y a}{2} \right), \quad (11)$$

$$S_\mu(\vec{q}) = \frac{2i\chi}{\sqrt{M}} \sin(q_\mu a). \quad (12)$$

From (9), the system of equations can be obtained in the quasimomentum representation:

$$i\hbar \frac{d\Phi(\vec{k})}{d\tau} = E(\vec{k}) \Phi(\vec{k}) + \frac{1}{\sqrt{N}} \sum_{\vec{q},\mu} S_\mu(\vec{q}) \Phi(\vec{k} - \vec{q}) Q_\mu(\vec{q}), \quad (13)$$

Fig. 1. Inverse radius of the localization, $1/R$, as a function of the coupling constant, g. The solid line corresponds to the numerical value for the system of discrete equations and the dot-dashed curve corresponds to the analytical estimate of $1/R(g)$ as the solution of Eq. (20)

$$\frac{d^2Q_\mu(\vec{q})}{d\tau^2} = -\Omega_\mu^2(\vec{q})Q_\mu(\vec{q}) - \frac{1}{\sqrt{N}}\sum_{\vec{k}} S_\mu^*(\vec{q})\Phi^*(\vec{k})\Phi(\vec{k}+\vec{q}). \tag{14}$$

From the last equation in the stationary case, we find the relation between the lattice and quasiparticle functions

$$Q_\mu(\vec{q}) = -\frac{S_\mu^*(\vec{q})}{\sqrt{N}\Omega_\mu^2(\vec{q})}\sum_{\vec{k}} \Phi^*(\vec{k})\Phi(\vec{k}+\vec{q}). \tag{15}$$

Substituting this result into (9) gives the following expression for the energy functional:

$$E_{tot} = \sum_{\vec{k}} E(\vec{k}) \mid \Phi(\vec{k}) \mid^2 \; - \frac{1}{2N}\sum_{\vec{k}} G(\vec{k}) \mid \wp(\vec{k}) \mid^2, \tag{16}$$

where

$$G(\vec{k}) = \sum_\mu \frac{|S_\mu(\vec{k})|^2}{\Omega_\mu^2(\vec{k})} = \frac{\chi^2}{w}\frac{\sin^2(k_x a)+\sin^2(k_y a)}{\sin^2\frac{k_x a}{2}+\sin^2\frac{k_y a}{2}}, \tag{17}$$

$$\wp(\vec{k}) = \sum_{\vec{q}} \Phi^*(\vec{q})\Phi(\vec{q}-\vec{k}) = \sum_{\vec{n}} e^{i\vec{k}\vec{n}}|\varphi_{\vec{n}}|^2. \tag{18}$$

Let us choose a trial function in the form of a localized lump

$$\Phi(\vec{k}) = \frac{\pi^2}{2N\kappa\tanh(\pi^2/2\kappa)} \times$$

$$\times \cosh^{-1}(\pi k_x a/2\kappa)\cosh^{-1}(\pi k_y a/2\kappa), \tag{19}$$

where κ, the width of the lump, is a variational parameter to be determined by minimizing the energy:

$$\frac{dE_{tot}(\kappa)}{d\kappa} = 0. \tag{20}$$

Note that a Gaussian function in [6, 8] and a decreasing exponential in [8, 9] have been used.

Next we substitute (19) into (16) and replace the sums over $\vec{k}$ by the corresponding integration. This gives us the following expression for the energy as a function of the localization parameter:

$$E_{\rm tot} = \mathcal{E}_0 - J\Big\{\frac{4\kappa}{\sinh(\kappa)}\tanh^{-1}(\tfrac{\pi^2}{2\kappa}) + g\varphi(\kappa)\times$$

$$\times\left[2\varphi(\kappa) + \left(\kappa\tanh^{-1}(\kappa)-1\right)\frac{\kappa}{\sinh^2(\kappa)}\right]\Big\}, \tag{21}$$

where

$$\varphi(\kappa) = \kappa\left[\tfrac{1}{6} - \tfrac{1}{\pi^2}e^{-\pi^2/\kappa}\left(1+\tfrac{1}{4}e^{-\pi^2/\kappa}\right)\right] -$$

$$-\frac{\pi^2 e^{-\pi^2/\kappa}}{2\kappa(1-e^{-\pi^2/\kappa})} + \log(1-e^{-\pi^2/\kappa}). \tag{22}$$

Here g is the dimensionless electron-phonon coupling constant,

$$g = \frac{2\chi^2 a^2}{Jw}. \tag{23}$$

In Fig.1, we present the plot of the inverse radius of the soliton, $1/R$, as a function of g determined by Eq. (20). The radius is determined using the definition

$$R^2 = \sum_{n,m}\left((n^2+m^2)|\varphi_{n,m}|^2\right) = -\tfrac{1}{a^2}\tfrac{d^2}{d\vec{k}^2}\wp(\vec{k})|_{\vec{k}=0}. \tag{24}$$

It follows from Eq.(20) that the localization takes place only when the nonlinearity constant g exceeds the critical value $g_{c1} \approx 6$.

In Fig.1, we also show the curve obtained by solving the static equations numerically. These results prove the existence of a critical value for g, below which no localization can take place and demonstrate that the value of g_{c1} predicted by the variational ansatz (19) is quite close to the actual one. Our expression gives a better fit to the numerical results than those obtained with a Gaussian or a decreasing exponential [8]. The chosen ansatz (19) also gives a reasonable prediction for the size of the soliton as long as the wave function is localized on at least a few lattice sites. Once the wave function is strongly localized, i.e., localized mostly on one lattice site, the approximation breaks down. In this case, the decreasing exponent gives a better fit [8].

Fig. 2. Energy corresponding to state (19), $E = (E_{tot}(\kappa) - \mathcal{E}_0)/J$, as a function of κ for (a) $g = 5.5 < g_{c1}$, (b) $g = 7$ ($g_{c1} < g < g_{c2}$), (c) $g = 12 > g_{c2}$, and (d) $g = 17$

The results of the energy calculations, using Eq. (21), (see Fig.2) suggest that there are three qualitatively different regimes depending on the value of the nonlinearity constant g. When $g < g_{c1}$, the energy minimum corresponds to a delocalized state with $\kappa = 0$ (see Fig.2,a), while the energy minimum is reached at a finite nonzero value of κ, which corresponds to the localization regime, when $g_{c1} < g < g_{c2}$ (Figs. 2,b and 2,c). The minimum of the energy shown in Fig.2, d is attained when $\kappa \to \infty$. This is the regime of strong localization, in which the localization occurs within one lattice site and corresponds to a small polaron state. At $g > g_{c2}$, the energy decreases monotonously with increase of κ, approaching its limiting value equal to the energy of the quasiparticle localized on one lattice site.

3. Modified Nonlinear Schrödinger Equation

In this section, we derive the dynamic equations of our discrete isotropic system and show their relation to the $2D$ NLSE. The dynamic equations in the site representation can be obtained in two ways: from the energy functional (5) or by using the inverse transformation (8) in Eq. (13).

From the results of the numerical simulations [7], we know that, for values of g not too small, the solutions are very smooth. Thus, it is appropriate to study the dynamic equations in the continuum approximation. For the static solutions, we can exclude deformational variables from the corresponding system of equations and derive the equation for the quasiparticle wavefunction in the form of a modified $2\,D$ NLSE:

$$i\frac{d\varphi}{d\tau} + \Delta\varphi + 2g\left(|\varphi|^2 + \frac{\alpha}{12}\Delta|\varphi|^2\right)\varphi = 0. \qquad (25)$$

Here the space coordinates are dimensionless, i.e., measured in lattice units, and the dimensionless time $\tau = Jt/\hbar$ has been introduced.

The continuum equation (25) can be obtained in different ways, the only difference is the numerical value of the coefficient of the last term, α, which is always relatively small, so that $\alpha/12 < 3$. Namely, within the

Fig. 3. *a* — numerical value of $1/R(g)$ for the system of discrete equations, *b* — the value of $1/R(g)$ obtained within the variational scheme for the continuum $2D$ MNLSE (25)

present scheme, according to (25), $\alpha = 1$; in the equation derived from the quasimomentum representation, $\alpha = 4$. While using the Taylor expansion in the site representation, one has $\alpha = 9/4$ (see [8]).

The conserved energy for Eq. (25), measured in units of J, is given by

$$\mathcal{E} = \int \left[|\vec{\nabla}\varphi|^2 - g|\varphi|^4 + \frac{g\alpha}{12} \left(\vec{\nabla}|\varphi|^2 \right)^2 \right] dxdy. \tag{26}$$

It is well known that the $2D$ NLSE,

$$i\frac{d\varphi}{d\tau} + \Delta\varphi + 2g|\varphi|^2\varphi = 0, \tag{27}$$

with the normalization condition (4) has a stationary solution only at a very specific value of the nonlinearity parameter; namely, at $g = 5.85$.

Moreover, this solution corresponds to the zero value of the total energy, while the localization parameter and binding energy can take arbitrary values. The solution of the $2D$ NLSE is marginally stable in the linear approximation [15] and is unstable with respect to perturbations of finite amplitude [10].

The extra term in Eq.(25), when compared with $2D$ NLSE (27), turns out to be essential for the stabilization of solitons. This comes from the fact that our model is defined on a lattice, which prevents the soliton collapse, as is shown below. Differentiating the square of the localization radius given by Eq. (24) with respect to τ (comp. [10, 16 — 18]), we find

$$\frac{dR^2}{d\tau} = -\int (x^2 + y^2)(\varphi\Delta\varphi^* - \varphi^*\Delta\varphi)dxdy, \tag{28}$$

which gives

$$\frac{d^2R^2}{d\tau^2} = 8(\mathcal{E} + \delta). \tag{29}$$

Here $\mathcal{E}$ is given by (26) and

$$\delta = \frac{g\alpha}{12} \int \left(\Delta|\varphi|^2 \right)^2 dxdy. \tag{30}$$

It follows from (29) that the initial configurations with negative energy $\mathcal{E}$ will start shrinking unless the extra term δ, which is always positive, can compensate $\mathcal{E}$. As a result of such shrinking, δ increases until the r.h.s. of (29) becomes negative. Then the wave function starts to expand until δ becomes small enough to make the soliton start to shrink again. This process continues, and, as a result, the soliton oscillates in size.

To estimate the oscillations, we consider the following Gaussian ansatz for the wave function

$$\varphi(x, y) = \frac{1}{\sqrt{\pi R^2}} \exp\left(-\frac{x^2+y^2}{2R^2} \right). \tag{31}$$

Substituting (31) into (26), we get the expression for the energy as a function of the localization parameter

$$\mathcal{E} = \frac{2\pi - g}{2\pi R^2} + \frac{g\alpha}{12\pi R^4}. \tag{32}$$

The minimum of the energy function is attained at a value for g that is slightly smaller than 6, which supports our analysis.

In Fig.3, we present the plot of $1/R(g)$ as a function of g together with the curve obtained numerically. We see that the curve fits the numerical value of $1/R$ quite well when g is not too large, i.e., when the continuum approximation is valid.

To study the stability of our solution, consider a state that differs slightly from the static solution; namely, we take

$$R^2 = R_0^2 + f(\tau), \tag{33}$$

where f is assumed to be small, and so, according to (29), satisfies the following equation:

$$\frac{d^2f(\tau)}{d\tau^2} = -\omega^2 f(\tau). \tag{34}$$

Here

$$\omega^2 = \frac{36}{\pi} \left(1 - \frac{2\pi}{g} \right)^3, \tag{35}$$

and, therefore, the size of the lump oscillates as a function of time:

$$R^2 = R_0^2 + \epsilon\cos(\omega\tau), \tag{36}$$

Fig. 4. Period of oscillation, $T(g)$, of the soliton width : a — numerical value; b — analytical estimate within the variational scheme: $T(g) = \frac{2\pi}{\omega} = \frac{1}{3}(\pi g/(g-2\pi))^{3/2}$

Fig. 5. The average soliton velocity, v_e, as a function of the wavevector, k, in dimensionless units. The top and bottom curves refer to the broader and narrower solitons, respectively

with the amplitude of oscillations, ϵ, determined by the initial conditions.

In Fig. 4, we present the curve $T(g) = 2\pi/\omega$ obtained by solving the initial discrete equations numerically and compare it with the values given by (35).

4. Moving Solitons

We have also studied numerically various properties of moving solitons. Such a system has been described by a set of discrete equations in the site representation (see [1]) on a 100×100 grid with periodic boundary conditions in the x direction. To make the solitons move, we have multiplied the quasiparticle wavefunction φ by a factor $e^{ik_x n_x}$, which accounts for the soliton momentum in the x direction and results in the soliton movement. As the soliton moves, it 'drags' the lattice deformation. This is achieved by the sharing of the momentum amongst the quasiparticle and the deformation of the lattice.

The relatively broad soliton moves around the effective cylinder several times without noticeable reduction of its velocity. This was observed for all sensible values of $k = k_x$ ($k \sim 0.01 - 0.5$) and $g \sim 6 - 7$. The soliton velocity v_e as a function of k is shown in Fig.5. The top and bottom curves in Fig.5 refer to the broader and narrower solitons, respectively. The narrower the soliton, the more momentum, k, it needs to move with the same velocity. This is due to the phonon dressing: the effective mass of the narrower soliton is larger than the mass of the broader one. The discreteness of the lattice manifests itself in two different ways. Firstly, in the deviation of the dispersion $v_e(k)$ from a linear relation to a curve with saturation.

To study this, we have introduced some absorption in the system and started off the soliton with a reasonable momentum.

In Fig. 6, we present the time dependence of the soliton velocity for two such cases. In case (a), we see that the soliton becomes trapped when the velocity drops below ~ 0.01, and its velocity oscillates around 0. In Fig. 6,b, the corresponding value is around ~ 0.005. Both cases describe relatively narrow solitons (the case (b) corresponds to the lower curve of Fig. 5). When we took a broader soliton, i.e., the one described by the upper curve of Fig. 5, we could not determine its very small critical velocity as the soliton had reflected itself from a lattice site and reversed its direction! At $v \sim 0.001$, the soliton was still moving very smoothly. Thus, we conclude that the discreteness can lead to some new coherent effects. Clearly, more work has to be done to understand these points better.

Fig. 6. Time dependence of the soliton velocity for relatively narrow trapped solitons. *a* — the critical velocity of trapping $v_{\rm cr} \sim 0.01$, *b* — $v_{\rm cr} \sim 0.005$ (the corresponding value of coupling is the same as for the lower curve of Fig. 5

Conclusions

We have shown that a $2D$ lattice where the electron-phonon interaction is taken into account admits solitonic solutions when the coupling constant g is larger than its lower critical value, $g_{c1} \approx 5.85$, and less than its upper critical value, $g_{c2} \approx 8$. In this interval a solitonic solution is stable with respect to finite and not too large perturbations. The stabilization of such a $2D$ soliton with respect to collapse occurs due to the mutual influence of nonlinearity, wave dispersion, and lattice discreteness. At $g > 8$, the self-trapping changes into the regime of strong localization. This transition also manifests itself by the bend of the numerical dependence $1/R(g)$, Fig.3. When the initial function is slightly different from the stationary state, its width oscillates around the value that corresponds to the width of the stationary state with the frequency of oscillations given by Eq. (35). The study of the dynamics of such a soliton and its stability with respect to collisions with boundaries is in progress.

Generally speaking, at various values of the electron-phonon coupling, different types of the electron ground state are realized: small polaron, soliton (large polaron), or almost free electron [19]. Between the almost free electron state at a weak coupling, and the small polaron state at a strong coupling there is a region of the coupling parameter, where a soliton state exists in systems that satisfy the adiabatic approximation. But the results of the zero adiabatic description of $1D$ and $2D$ systems with respect to the self-trapping are qualitatively different. While in 1DSs within the adiabatic approximation, the self-trapping *formally* occurs at an arbitrary value of the coupling constant, in 2DS systems even within the adiabatic approximation, there are three different regimes which can be realized depending on the strength of the coupling.

The comparison of the results obtained here with the conditions of the soliton existence in $1D$ chains [19] shows that solitons in $2D$ lattices exist at larger values of the electron-phonon coupling constant. Therefore, the properties of systems of similar compounds but possessing a $1D$ rather than a $2D$ structure, could differ qualitatively. Indeed, such an example is given by the comparative study of the vibrational modes of the double $C = O$ bond of a peptide group, called Amide-I vibrational modes, in biological macromolecules of myoglobin and in photoactive yellow protein, respectively [20]. Myoglobin, which is essentially α-helical, i.e., is a quasi-$1D$ protein, admits the existence of a long-lived photoexcited Amide-I mode with lifetime greater than 15 ps. On the other hand, photoactive yellow protein, which is predominantly a β-sheet protein, does not have such long-lived modes under the same conditions of photoexcitation. Let us add here that A.S. Davydov and N.I. Kislukha [21] were the first to predict the self-trapping of Amide-I excitations in a soliton state in α-helical macromolecules due to the electron-phonon coupling with the hydrogen bonds along polypeptide chains, the life-time of such a soliton state being much higher than that of an isolated Amide-I excitation [14].

In this paper, we have also presented the preliminary results of a numerical study of moving solitons in 2 D lattices. We have shown that solitons, once formed, can move and lose a little energy when moving. This is particularly true for broad solitons; narrower solitons 'feel' the effects of the lattice more and can get trapped on lattice sites.

The authors express their thanks to Professor T.A. Davydova for stimulating discussions.

The work reported here, was partly supported by the Project No. 0102U002332 of the Fundamental Research Programme of the Ukrainian NASc. A travel grant from NATO is also acknowledged.

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Received 15.03.02

АВТОЛОКАЛІЗАЦІЯ ЕЛЕКТРОНІВ У ДИСКРЕТНИХ ДВОВИМІРНИХ ГРАТКАХ.
II. АНАЛІТИЧНЕ ДОСЛІДЖЕННЯ

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У попередній роботі [1] нами було досліджено чисельно автолокалізовані електронні стани у дискретних анізотропних двовимірних електрон-фононних гратках. Тут ця проблема досліджується аналітично у випадку ізотропних граток. Показано, що в адіабатичному наближенні система дискретних рівнянь може бути зведена до континуального двовимірного нелінійного рівняння Шредінгера з додатковим доданком, що виникає завдяки дискретності і є істотним для протидії колапсу солітонів. Це досягається тоді, коли параметр нелінійності набуває значення з певного інтервалу $g_{c1} < g < g_{c2}$. Варіаційним методом показано, що мінімум енергії відповідає делокалізованим станам, коли $g < g_{c1}$, та сильно локалізованим (майже на одному вузлі) при $g > g_{c2}$. Розраховано радіус локалізації квазічастинки як функцію сталої електрон-фононної взаємодії. Наведено також деякі результати стосовно солітонів з відмінною від нуля швидкістю.

АВТОЛОКАЛИЗАЦИЯ ЭЛЕКТРОНОВ В ДИСКРЕТНЫХ ДВУМЕРНЫХ РЕШЕТКАХ.
II. АНАЛИТИЧЕСКОЕ ИССЛЕДОВАНИЕ

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В предыдущей работе [1] нами были численно исследованы автолокализованные электронные состояния в дискретных анизотропных двумерных электрон-фононных решетках. Здесь эта проблема исследуется аналитически в случае изотропных решеток. Показано, что в адиабатическом приближении система дискретных уравнений может быть сведена к континуальному двумерному нелинейному уравнению Шредингера с дополнительным слагаемым, которое появляется из-за дискретности и оказывается существенным для противодействия коллапсу солитонов. Это достигается тогда, когда параметр нелинейности принимает значения из определенного интервала $g_{c1} < g < g_{c2}$. Вариационным методом показано, что минимум энергии соответствует делокализованным состояниям, когда $g < g_{c1}$, и сильно локализованным (в пределах одного узла) при $g > g_{c2}$. Рассчитан радиус локализации квазичастицы как функция постоянной электрон-фононного взаимодействия. Представлен также ряд результатов, касающихся движущихся солитонов.