SOLITONIC STATES AND NONLINEAR SCHRÖDINGER EQUATION IN TWO AND MORE DIMENSIONS

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In this talk, I present and discuss some results of [1—4] and [5]. In these papers we have shown that, for a suitable range of parameters, the two-dimensional discrete equations describing a quasiparticle interacting with the displacements of a lattice of atoms possess solitonic solutions. We also show that, in the continuum limit, the effective equation for the quasiparticle reduces to the nonlinear and, in general, nonlocal Schrödinger equation. We describe the conditions when this equation also possesses solitonic solutions. We discuss some further generalizations of this problem.

1. Introduction

Depending on their strength, the electron-phonon interactions in systems involving electrons moving in deformable lattices of atoms can become very important for the dynamics of such systems and may lead to some very interesting phenomena. An example of such a phenomenon is the quasiparticle self-trapping which is sometimes referred to as spontaneous or the auto-localization of a quasiparticle. In fact, Davydov [6, 7] already in 1973 suggested that such a self-trapping of Amide-I excitations takes place in one-dimensional proteins. Thus, it is interesting to perform a comparative study of systems with similar chemical composition and those belonging to different classes. In [8], an example of such a system was given; it was shown there that the life-time of Amide-I excitation in myoglobin is much higher than the life-time of the excitations of photoactive yellow protein.

It is also known that, in effectively one-dimensional systems, a quasiparticle (electron, hole, exciton, etc) self-trapping takes place only for a particular range of values of the parameters characterizing the system [9]. A similar, although somewhat more complex, situation exists also for two-dimensional systems. Thus, in particular, it has been shown in [1, 2] that the self-trapped solitonic states of a quasiparticle exist and are stable both in isotropic and anisotropic two-dimensional crystals within some intervals of numerical values of the relevant parameters.

Many one-dimensional systems, such as polypetides, etc., have been shown to possess acoustic and optical phonons and to admit the existence of Davydov or molecular solitons. This derivation is based on the adiabatic approximation which results in nonlinear and/or coupled equations which are then studied numerically. When one considers their continuum limit, the equations describing the collective excitations of such systems reduce to a one-dimensional nonlinear Schrödinger equation with an attractive interaction. Such systems have attracted much interest and have been studied by various people. So far, however, relatively little attention has been paid to higher dimensional systems where, of course, the spectrum of possibilities is much richer as the systems can be anisotropic.

Here we report some results of our attempts to perform such investigations (of two-dimensional systems) [1—5]. And given that the original ideas go back to the seminal work of Davydov [6], it gives me particular pleasure to give this talk at this conference dedicated to the 90th anniversary of A.S. Davydov and held in his Institute.

2. Hamiltonian of the System

In [1, 2], we have considered systems which are described by the Hamiltonian which is the sum of Hamiltonians describing the electron, phonons and electron-phonon interactions:

$$\hat{H} = \hat{H}_e + \hat{H}_{\rm ph} + \hat{H}_{\rm int}. \quad (1)$$

These Hamiltonians, in the site representation, are given by:

$$\hat{H}_e = \sum_{m,n}[\mathcal{E}_0 A^+_{m,n}A_{m,n} - j_x(A^+_{m,n}A_{m+1,n}+$$

$$+A^+_{m+1,n}A_{m,n}) - j_y(A^+_{m,n}A_{m,n+1} + A^+_{m,n+1}A_{m,n})], \quad (2)$$

$$\hat{H}_{\rm ph} = \tfrac{1}{2}\sum_{m,n}\Big(\frac{\hat{p}^2_{m,n}}{M} + \frac{\hat{q}^2_{m,n}}{M} + k_x\,[(\hat{u}_{m,n} - \hat{u}_{m+1,n})^2+$$

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$$+(\hat{v}_{m,n}-\hat{v}_{m+1,n})^2]+k_y\,[(\hat{u}_{m,n}-\hat{u}_{m,n+1})^2+$$

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

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

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

Here $A^+_{m,n}$ ($A_{m,n}$) denote the creation (annihilation) operators of the electron at the site (m,n), $\hat{u}_{m,n}$, $\hat{v}_{m,n}$ and $\hat{p}_{m,n}$, $\hat{q}_{m,n}$ are the longitudinal and transverse components of the vector operator of molecule displacements and their respective conjugated momenta. The energy $\mathcal{E}_0-2j_x-2j_y$ corresponds to the bottom of the electron energy band; the constants j_x, j_y are the exchange interaction energies, while χ_x, χ_y stand for the electron-phonon coupling constants in the x and y directions, respectively. Finally, k_x, k_y are the corresponding lattice elasticity coefficients.

$\hat{H}_{\rm int}$, the Hamiltonian of the electron-phonon interaction, is taken in the simplest form [6] and so it involves only the "nearest neighbour" interaction between the electron field and the deformation of the lattice. Later, we shall discuss some generalizations of this assumption.

To proceed further, we perform the standard semiclassical analysis and derive the effective classical Hamiltonian H with $\varphi_{m,n}$ describing the probability amplitude of the electron, and $u_{m,n}$, $v_{m,n}$ are the classical variables describing molecular displacements from their positions of equilibrium, respectively, in the x and y directions.

The effective Hamiltonian is then given by

$$H=\sum_{m,n}((\mathcal{E}_\prime+\mathcal{W})\,|\varphi_{m,n}|^2-j_x\,\varphi^*_{m,n}(\varphi_{m+1,n}+$$

$$+\varphi_{m-1,n})-j_y\,\varphi^*_{m,n}(\varphi_{m,n+1}+\varphi_{m,n-1})+|\varphi_{m,n}|^2\times$$

$$\times\big[b\chi_x\,(u_{m+1,n}-u_{m-1,n})+a\chi_y\,(v_{m,n+1}-v_{m,-1})\big], \tag{5}$$

where W describes the phonon energy and is given by

$$\mathcal{W}=\tfrac{1}{2}\sum_{m,n}\Big(\frac{p^2_{m,n}}{M}+\frac{q^2_{m,n}}{M}+k_x\,[(u_{m,n}-u_{m+1,n})^2+$$

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

$$+(v_{m,n}-v_{m,n+1})^2]\Big). \tag{6}$$

Our set of equations involves also a constraint: the electron function must satisfy the normalization condition, which in our case takes the form:

$$\sum_{m,n}|\varphi_{m,n}|^2=1. \tag{7}$$

This normalization condition is not very important in one dimension for one electron. However, it becomes essential in many-electron problems in 1-dimensional systems and it leads to nontrivial effects in the 2-dimensional lattice cases even for just one electron.

Next, to simplify all the formulae, we introduce the dimensionless variables

$$\tau=\frac{j_x t}{\hbar},\quad U=C_x\,\frac{u}{b},\quad V=C_x\,\frac{v}{b},\quad E_s=\frac{b^2 M j_x}{\hbar^2},$$

$$E_0=\frac{\mathcal{E}_\prime}{j_x}, C_x=\frac{\chi_x\,b^2}{j_x},\quad C_y=\frac{\chi_y\,a\,b}{j_x},$$

$$K_x=\frac{k_x\,\hbar^2}{M\,j_x^2},\quad K_y=\frac{k_y\,\hbar^2}{M\,j_x^2},\quad g=\frac{2\,C_x^2}{K_x\,E_s}$$

and also the anisotropy parameters

$$A_j=\frac{j_y}{j_x},\qquad A_c=\frac{C_y}{C_x},\qquad A_k=\frac{K_y}{K_x}. \tag{8}$$

It is easy to derive the Euler—Lagrange equations describing the dynamics of our system. They are given by

$$i\,\tfrac{d\varphi_{m,n}}{d\tau}=(E_0+W)\,\varphi_{m,n}-(\varphi_{m+1,n}+\varphi_{m-1,n})-$$

$$-A_j\,(\varphi_{m,n+1}+\varphi_{m,n-1})+\big[(U_{m+1,n}-U_{m-1,n})+$$

$$+A_c\,(V_{m,n+1}-V_{m,n-1})\big]\,\varphi_{m,n}, \tag{9}$$

$$\tfrac{d^2U_{m,n}}{d\tau^2}=-\frac{K_x}{C_x}\,\big[(2\,U_{m,n}-U_{m+1,n}-U_{m-1,n})+$$

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

$$-\frac{g}{2}\,(|\varphi_{m+1,n}|^2-|\varphi_{m-1,n}|^2)\big], \tag{10}$$

$$\tfrac{d^2V_{m,n}}{d\tau^2}=-\frac{K_x}{C_x}\,\big[(2\,V_{m,n}-V_{m+1,n}-V_{m-1,n})+$$

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

$$-\frac{g\,A_c}{2}\,(|\varphi_{m,n+1}|^2-|\varphi_{m,n-1}|^2)\big], \tag{11}$$

with the phonon energy given by

$$W=\tfrac{1}{2}\,E_s\sum_{m,n}\Big(P^2_{m,n}+Q^2_{m,n}+$$

$$+\frac{K_x}{C_x}\left([(U_{m,n}-U_{m+1,n})^2+(V_{m,n}-V_{m+1,n})^2]+\right.$$

$$\left.+A_k[(U_{m,n}-U_{m,n+1})^2+(V_{m,n}-V_{m,n+1})^2]\right), \qquad (12)$$

where

$$P_{m,n}=\frac{dU_{m,n}}{d\tau}, \quad Q_{m,n}=\frac{dV_{m,n}}{d\tau}. \qquad (13)$$

Clearly, equations (2.10) — (2.12) are very hard to solve, so we have studied them numerically in [1—4]. In the next section, we describe some results of these studies.

3. Numerical Results

First, we have looked at the stationary solutions of our equations. We have done this in many ways, in particular by adding "absorptive" terms to equations (2.11) and (2.12) and by using various initial configurations.

In the isotropic case, we have found that, for $g > g_{\rm cr} \sim 5.85$, we have localized solitons (i.e., solitonic configurations) with the φ field being the most strongly localized. As g increases, the solitons become more and more localized and, for $g \sim 20$, the solitons are localized to within a very few lattice sites. For g close to $g_{\rm cr}$, the solitons are quite broad and, for $g < g_{\rm cr}$, the equations do not have stationary localized solutions. When one attempts to find a localized solution (by starting a numerical simulation with a soliton-like initial configuration), the fields spread out over the whole lattice.

Similar results hold also in anisotropic cases. All details of our results and various plots of the field configurations and of the corresponding energy densities can be found in [1].

Can we understand our numerical results?

4. Narrow Solitons

Let us restrict our attention to the isotropic case (for a discussion of anisotropic cases, see [1] and [2]). Hence, we can put $A_j = A_k = A_c = 1$. Next we define

$$\Delta(1)U_{m,n} = 4U_{m,n} - U_{m+1,n} - U_{m-1,n} -$$

$$-U_{m,n+1} - U_{m,n-1} \qquad (14)$$

and

$$\Delta(2)|\varphi_{m,n}|^2 = 4|\varphi_{m,n}|^2 - |\varphi_{m+2,n}|^2 - |\varphi_{m-2,n}|^2 -$$

$$-|\varphi_{m,n+2}|^2 - |\varphi_{m,n-2}|^2. \qquad (15)$$

Noting that, as $A_k = 1$, the equations for the static U and V fields can be rewritten as

$$\Delta(1)(U_{m+1,n} - U_{m-1,n}) = \tfrac{g}{2}(|\varphi_{m+2,n}|^2 - |\varphi_{m,n}|^2 -$$

$$-|\varphi_{m,n}|^2 + |\varphi_{m-2,n}|^2), \qquad (16)$$

$$\Delta(1)(V_{m,n+1} - V_{m,n-1})0 = \tfrac{g}{2}(|\varphi_{m,n+2}|^2 - |\varphi_{m,n}|^2 -$$

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

and so we have

$$\Delta(1)\left((U_{m+1,n} - U_{m-1,n}) + (V_{m,n+1} - V_{m,n-1})\right) =$$

$$= -\tfrac{g}{2}\Delta(2)|\varphi_{m,n}|^2. \qquad (18)$$

Thus, we have obtained a very **interesting equation**

$$\Delta(1)Z_{m,n} = -\tfrac{g}{2}\Delta(2)|\varphi_{m,n}|^2, \qquad (19)$$

where

$$Z_{m,n} = (U_{m+1,n} - U_{m-1,n}) + (V_{m,n+1} - V_{m,n-1}). \qquad (20)$$

In (19), $\Delta(1)$ describes a 5-point Laplacian and $\Delta(2)$ is the same operator but, effectively, missing out the nearest points of the lattice (i.e., an operator on a lattice twice as large) as described in (15) and (16). Unfortunately, we have not been able to solve this discrete equation exactly except in one dimension — (i.e., for a 3-point Laplacian). In this one-dimensional case, the equation becomes

$$P_{i+1} + P_{i-1} - 2P_i = \kappa(2R_i - R_{i+2} - R_{i-2}) \qquad (21)$$

and is solved by

$$P_n = -\kappa(R_{n+1} + R_{n-1} + 2R_n), \qquad (22)$$

where we have neglected the boundary terms.

To solve our equations in two dimensions, we look first at the eigenvalue equation for φ:

$$-\lambda\varphi_{m,n} = -(\varphi_{m+1,n} + \varphi_{m-1,n} + \varphi_{m,n+1} + \varphi_{m,n-1} -$$

$$-4\varphi_{m,n}) + Z_{m,n}\varphi_{m,n}, \qquad (23)$$

where $Z_{m,n}$ defined by (20) satisfies (19). We attempt to solve this equation iteratively. Thus, first we assume that $|\varphi_{0,0}|^2 = 1$ and set all other $|\varphi_{m,n}|^2$ zero. We find

$$Z_{0,0} = -\tfrac{8}{11}g, \qquad Z_{1,0} = -\tfrac{5}{22}g, \qquad Z_{1,1} = -\tfrac{4}{33}g,$$

$$Z_{2,0} = \tfrac{2}{33}g, \qquad Z_{2,1} = -\tfrac{1}{66}g. \qquad (24)$$

Then we use this result to determine a "new-modified" φ_{ij}. So we assume

$$\varphi_{0,0} = 1 - \tfrac{F}{g^2}, \qquad \varphi_{m,n} = f_{m,n}\, g^{-(|m|+|n|)}. \tag{25}$$

Moreover, we impose

$$f_{m,n} = f_{|m|,|n|}. \tag{26}$$

Then we find

$$\lambda = -4 + \tfrac{8}{11}g, \qquad f_{1,0} = 2,$$

$$f_{1,1} = \tfrac{33}{5}, \qquad f_{2,0} = \tfrac{33}{13}, \qquad F = 8, \tag{27}$$

which is, in fact, in a good agreement with the solutions determined numerically! The detailed comparisons are given in [1].

5. Broad Solitons

When the coupling constant g is small (but larger than $g_{\rm cr}$) we expect the continuum limit approximation to be valid. To construct this approximation, we define $\varphi(x,y) = \varphi_{m,n}$ as functions of the continuous variables x and y instead of the discrete variables m and n. Then, using the Taylor expansion

$$\varphi_{m\pm1,n} = \varphi_{m,n} \pm \tfrac{\partial\varphi(x,y)}{\partial x} + \tfrac{1}{2}\tfrac{\partial^2\varphi(x,y)}{\partial x^2} \pm \tfrac{1}{6}\tfrac{\partial^3\varphi(x,y)}{\partial x^3} + \ldots, \tag{28}$$

$$U_{m\pm1,n} = U_{m,n} \pm \tfrac{\partial U}{\partial x} + \tfrac{1}{2}\tfrac{\partial^2 U}{\partial x^2} \pm \tfrac{1}{6}\tfrac{\partial^3 U}{\partial x^3} + \tfrac{1}{24}\tfrac{\partial^4 U}{\partial x^4} + \ldots, \tag{29}$$

$$V_{m,n\pm1} = V_{m,n} \pm \tfrac{\partial V}{\partial y} + \tfrac{1}{2}\tfrac{\partial^2 V}{\partial x^2} \pm \tfrac{1}{6}\tfrac{\partial^3 V}{\partial x^3} + \tfrac{1}{24}\tfrac{\partial^4 V}{\partial x^4} + \ldots, \tag{30}$$

we can write

$$\tfrac{\partial^2 U}{\partial x^2} = -g\left(\tfrac{\partial|\varphi|^2}{\partial x} + \tfrac{1}{6}\tfrac{\partial^3}{\partial x^3}|\varphi|^2\right), \tag{31}$$

$$\tfrac{\partial^2 V}{\partial y^2} = -g\left(\tfrac{\partial|\varphi|^2}{\partial y} + \tfrac{1}{6}\tfrac{\partial^3}{\partial y^3}|\varphi|^2\right), \tag{32}$$

where we have neglected $\frac{\partial^2 U}{\partial y^2}$ and $\frac{\partial^2 V}{\partial x^2}$. Integrating (31) and (32) and setting all the "constants of integration" to zero, we get

$$\tfrac{\partial U}{\partial x} = -g\left(|\varphi|^2 + \tfrac{1}{6}\tfrac{\partial^2}{\partial x^2}|\varphi|^2\right), \tag{33}$$

$$\tfrac{\partial V}{\partial y} = -g\left(|\varphi|^2 + \tfrac{1}{6}\tfrac{\partial^2}{\partial y^2}|\varphi|^2\right). \tag{34}$$

So the equation for φ becomes

$$i\tfrac{d\varphi}{d\tau} + \Delta\varphi + 2g\left(|\varphi|^2 + \tfrac{1}{12}\Delta|\varphi|^2\right)\varphi = 0, \tag{35}$$

i.e., a **Nonlinear Schrödinger Equation** with an extra term.

Clearly, had we neglected the last term in (35) and so used only the Schrödinger equation

$$i\tfrac{d\varphi}{d\tau} + \Delta\varphi + 2g|\varphi|^2\varphi = 0, \tag{36}$$

its solutions would be unstable. But we have this extra term which comes from the lattice and stabilizes solitons. To get a better understanding of this effect, we consider first the square of the size of any localized, soliton-like, configuration

$$R^2 = \int |\varphi(x,y)|^2 (x^2+y^2)\,dxdy. \tag{37}$$

Differentiating with respect to τ and using (35), we get:

$$\tfrac{dR^2}{d\tau} = -\int (x^2+y^2)(\varphi\Delta\varphi^* - \varphi^*\Delta\varphi)\,dxdy. \tag{38}$$

So we see that

$$\tfrac{d^2R^2}{d\tau^2} = 8(\mathcal{E}+\delta), \tag{39}$$

where

$$\mathcal{E} = \int \left[|\vec{\nabla}\varphi|^2 - g|\varphi|^4 + \tfrac{g}{12}\left(\Delta|\varphi|^2\right)^2\right] dxdy \tag{40}$$

and

$$\delta = \tfrac{g}{12}\int \left(\Delta|\varphi|^2\right)^2 dxdy. \tag{41}$$

Note that, as $\mathcal{E} < 0$ and $\delta > 0$, the interplay between these two terms produces a behaviour which alternates between shrinking and expanding and thus leads to the stabilization of a soliton.

To get a better "feeling" for the existence of a solitonic solution, we approximate φ by a Gaussian function (which, in fact, is not a bad approximation). Thus, we consider

$$\varphi(x,y) = \frac{\kappa}{\sqrt{\pi}}\,\exp\left(-\frac{\kappa^2}{2}(x^2+y^2)\right) \tag{42}$$

and then insert it into (40). We find that

$$\mathcal{E} = \kappa^2\left(1 - \frac{g}{2\pi}\right) + g\frac{\kappa^4}{12\pi}. \tag{43}$$

So we see that the value of κ minimizing $\mathcal{E}$ is given by

$$\kappa_0^2 = 3\left(1 - \frac{2\pi}{g}\right). \tag{44}$$

Looking at this result, we note the existence of a critical value $g_c = 2\pi$ below which there is no stable solution. Let us recall that when we had solved (10-12) numerically, we have found $g_{\rm cr} \approx 5.85$, which is clearly not very different from 2π.

6. Further Comments

Our Gaussian approximation, though good, is not perfect. The question then arises as to whether we can find a better approximation. We have, in fact, tried various functions [2]. Thus, we have considered approximating the electron function by (all in the momentum space)

(i) a Gaussian function

$$\Phi(\vec{k}) = \frac{A_1}{N} \exp\left\{-\frac{a^2}{2\kappa^2}\left(k_x^2 + k_y^2\right)\right\},$$

(ii) a decreasing exponent

$$\Phi(\vec{k}) = \frac{A_2}{N} \sum_{\vec{k}} \exp\left(-\kappa(|n_x| + |n_y|)\right) \exp\left(-i\vec{k}\vec{n}a\right),$$

(iii) a hyperbolic secant

$$\Phi(\vec{k}) = \frac{A_3}{N} \cosh^{-1}\left(\pi k_x a/2\kappa\right) \cosh^{-1}\left(\pi k_y a/2\kappa\right),$$

and (iv) elliptic functions

$$\Phi(\vec{k}) = \Phi(k_x)\Phi(k_y), \quad \Phi(k_\mu) = \frac{2A_4 K(k)}{\pi\sqrt{N}} dn(u_\mu, k),$$

where $A_i, i = 1, .., 4$ are normalization coefficients, $dn(u_\mu, k)$ are elliptic Jacobi functions, and $u_\mu = K(k)ak_\mu/\pi$, where $K(k)$ is the complete elliptic integral of the first kind.

All these approximations have produced qualitatively similar results, as has been discussed in [2] with the elliptic approximation being, perhaps, the best (i.e., the closest to the numerical solution).

We have also studied moving solitons. To do this, we have introduced periodic boundary conditions and boosted the field φ by multiplying it by the phase factor $\exp(ikx)$. Our studies have shown that such solutions do exist and that the U and V fields get "dragged" by the φ field. Of course, there is a relation between k and v, the velocity of the soliton. Moreover, the lattice coarseness effects lead to the existence of a critical velocity (which depends on g) below which the soliton is trapped at a lattice site.

When we have studied the scattering of two-solitons, we have found them to be robust (i.e., scattering off each other without changing a shape) except for essentially "head-on" collisions in some cases. In these cases, for a relatively small range of g, the solitons tended to stick together forming a new very narrow "double soliton".

However, as our two-soliton Hamiltonian had no Coulomb repulsion terms, our results are not very physical as they describe interactions of chargeless states.

7. Modified NLSE in D Dimensions

Given the reduction of our equations to the modified NLSE, we have decided to study this equation in more detail. Here we reproduce some of the results in [3], where we have considered the problem, in general, in D dimensions. Thus, we have studied the equation

$$i\varphi_t + \Delta\varphi + 2\left(g|\varphi|^2 + G\Delta|\varphi|^2\right)\varphi = 0, \tag{45}$$

where G is a "new" coupling constant which was set to $\frac{g}{12}$ in the previously considered case.

First, we note that this equation has several conserved quantities; namely:

1) the norm functional

$$N = \int dx^D |\varphi|^2, \tag{46}$$

2) energy (already mentioned in (40))

$$H = \int dx^D \left(|\vec{\partial}\varphi|^2 - g|\varphi|^4 + G(\vec{\partial}|\varphi|^2)^2\right), \tag{47}$$

3) momentum

$$\vec{I} = \int dx^D \vec{j}, \qquad j_\mu = -\frac{i}{2}\left(\varphi^* \frac{\partial\varphi}{\partial x_\mu} - \varphi\frac{\partial\varphi^*}{\partial x_\mu}\right), \tag{48}$$

and

4) angular momentum

$$L_{\mu\nu} = \int dx^D \left(x_\mu j_\nu - x_\nu j_\mu\right). \tag{49}$$

It is convenient to define also the **eigenenergy**

$$\Lambda = \int dx^D \frac{i}{2}\left(\varphi^* \frac{\partial\varphi}{\partial t} - \varphi\frac{\partial\varphi^*}{\partial t}\right). \tag{50}$$

Then, for a solution of the form (stationary solution)

$$\varphi = \phi e^{-i\lambda t}, \tag{51}$$

we find that

$$\Lambda = \lambda N. \tag{52}$$

For a soliton to exist, we need (for stability) $H < 0$ (and not necessarily $\Lambda < 0$). Note that H and Λ are related but **not** equal to each other.

Then, our results given in [3] have shown that:

- The equation has solitonic solutions for $g > g_{\rm cr}$.
- $g_{\rm cr}$ depends on D (dimension) and its value increases with D.

Critical values $g_{\rm cr}$ determined numerically and by a Gaussian ansatz

D	Numerical $g_{\rm cr}$	Ansatz $g_{\rm cr}$
2	5.85	$2\pi \approx 6.2832$
3	26.4094	$3\pi(5\pi/2)^{1/2} \approx 26.4129$
4	82.6714	$8\pi^2 \approx 78.957$
5	254.964	$5(\pi)^{5/2}(35/18)^{3/2} \approx 237.16$

In Table, we present our results on the value of $g_{\rm cr}$ determined numerically and estimated by a Gaussian ansatz. In this calculation, $G = g$. As we see, the agreement between the two expressions is amazingly good.

More details are given in [3].

Here we finish by adding a few comments:

- As g increases — solitons are narrower and more bound (the energy is more negative).
- In each case, a good approximation is given by a Gaussian ansatz.
- There exist further unstable solutions (which become stable as g increases).
- At $D = 2$, there exist also states with nonzero angular momentum l. Their $g_{\rm cr}$ also increases with the value of l.
- Soliton can be made to move — so we can study their dynamics.

8. More General Interactions

In this section, we return to our original problem discussed in Section 2. There, in the one-dimensional case, we considered the interaction Hamiltonian given by

$$\hat{H}_{\rm int} = \chi \sum_i A_i^\dagger A_i \, (\hat{U}_{i+1} - \hat{U}_{i-1}). \tag{53}$$

Let us now generalize this interaction further by considering

$$\hat{H}_{\rm int} = \sum_{ij} A_i^\dagger A_i \, K_{ij} \hat{U}_j, \tag{54}$$

where K_{mn} is a function which controls the number of lattice points involved (if we go beyond the "nearest neighbour" approximation). Then the final total (one-dimensional) Hamiltonian (in the adiabatic approximation) is given by

$$\hat{H} = \sum_m \left[\frac{P_m^2}{2M} + \kappa (U_m - U_{m+1})^2 - \right.$$

$$\left. - \sum_l J_{lm} \phi_m^\dagger \phi_l + \text{c.c} + \sum_k K_{mk} |\phi_m|^2 \, U_k \right], \tag{55}$$

where J_{lm} allows for going beyond the "nearest neighbour" approximation also in the couplings of the electron field.

Now the equations of motion take the form:

$$i \frac{d\phi_m}{dt} = E\phi_m - \sum_l J_{lm} \phi_l - \sum_k K_{mk} \phi_m U_k \tag{56}$$

and

$$\frac{d^2 U_m}{dt^2} = \kappa (2U_m - U_{m+1} - U_{m-1}) + \sum_k K_{km} |\phi_k|^2. \tag{57}$$

The second equation is really the spatially discretized version of

$$\Box U_m = P_m \tag{58}$$

and so has a solution:

$$U_m = \sum_n G_{mn} \, P_n, \tag{59}$$

where G_{mn} is the appropriate Green's function.

Thus, we see that

$$U_m = \sum_{nk} G_{mn} \, K_{kn} \, |\phi_k|^2 = \sum_k \tilde{G}_{mk} \, |\phi_k|^2 \tag{60}$$

and so, after some redefinitions,

$$i \frac{d\phi_m}{dt} = E\phi_m -$$

$$- \sum_l J_{lm} \phi_l - \sum_k K_{mk} \phi_m \sum_l \tilde{G}_{kl} |\phi_l|^2 =$$

$$= E\phi_m - \sum_l J_{lm} \phi_l - \sum_r Z_{mr} \, \phi_m |\phi_r|^2. \tag{61}$$

Note that the last term in our ϕ equation comes from

$$V(|\phi|^2) = \sum_{mr} Z_{mr} \, |\phi_m|^2 \, |\phi_r|^2, \tag{62}$$

i.e., which is a *nonlocal* $\lambda\phi^4$ potential.

Thus, we have shown that, in general, the interactions with the lattice generate nonlinear and nonlocal potentials. The specific form of the nonlocality is determined by details of the interaction between the electron field and deformations of the lattice.

Let us finish this section by observing that this discussion generalizes to higher dimensions. Moreover, we can present a different derivation based on the original equations (i.e., before performing the adiabatic approximation).

9. Other Deformations

Recently, Gaididei et al. [10, 11] have done some work on the study of curvature-induced symmetry breaking effects in nonlinear Schrödinger models. Their idea was to study a one-dimensional discrete Nonlinear Schrödinger equation

$$i\frac{d}{dt}\psi_i + \sum_k J_{ik}\,\psi_k + \chi|\psi_i|^2\psi_i = 0 \qquad (63)$$

in which the excitation transfer function (J_{ik}) depends on the positions of lattice points. Normally, one restricts oneself to the nearest neighbour approximation in which case $J_{ik} = J\delta_{i-k,\pm 1}$ but, as pointed out in [10], a more general case involves $J_{ik} = J(|\vec{r_i} - \vec{r_k}|)$ where $\vec{r_i}$ describes the spatial position of the ith lattice site. Of course, one would expect $J(|\vec{r_i} - \vec{r_k}|)$ to be a fast decreasing function of its argument. When all the points of the lattice lie along a straight line, i.e. $\vec{r_i} = \vec{a} + \alpha_i\vec{b}$, where α_i is a linearly growing function of i, the results are not that different from the case of a regular lattice with the nearest neighbour approximation. However, as pointed out in [10], any curvature in $\vec{r_i}$ can induce extra effects which do affect the behaviour of the ψ fields.

This idea comes from the study of the dynamics of biopolymers [11]. The authors of [11] have considered the case of an electron-like field on one polymer chain. The links of the polymers have been allowed to move, and their motion has been controlled by their interlink forces and also by the force due to the electron field. However, this model can also be considered as a further generalization of the models studied in the previous sections.

In the work reported in [11], one end of the polymer has been set to be free; the other one, assumed to be far away, has been kept fixed. The authors of [11] then have performed many interesting simulations of the equations which govern the dynamics of the electron and the lattice. Their most spectacular results have involved them showing that a single excitation of the ψ field at the free end results, after a long period of time, in a gradual folding of the chain. Then they have explained their results as coming from the instability generated by the development of the curvature of the chain.

These exciting results have made us think of systems involving more chains with an interchain interaction. Thus, we have decided to extend the investigations of [11] to systems of two chains with the simplest interchain interaction as given in, e.g., [12] and inspired by the Morse potential [13]. So we have looked at a system of two chains with coupling constants given by the appropriate generalizations of those of [11]. Note that the coupling between the electron fields on two chains allows the field to spread between them altering the values of the effective coupling constants on each chain.

Our results are still very preliminary as the work is still in progress [5]. However, we see at this stage that we have not reproduced Gaididei et al. [11] results (in detail) but have found similar soliton behaviour. We have also found that when, initially, the excitation is located at the first point of the chain — it generates a moving soliton. For solitons, we have found that their speed increases but the height decreases as β gets smaller. The first results for two chains have found a strong dependence on the interchain potential. The simulations have shown somewhat exotic behaviour but as these are only preliminary results we do not report them here.

Conclusions and Further Comments

In this talk, we have given the overview of our recent results [1—5]. We have shown that our discrete model, for a range of parameters, possesses solutions which are solitonic in nature. The model, in its continuum limit, becomes a **modified** nonlinear Schrödinger model and, in the most general case, leads to a nonlocal version of this model. The details of the nonlocality depend on the coupling between the electron field and deformations of the lattice.

The nonlocality, in the specific cases studied by us, is responsible for the existence of solitons. We have also analyzed our modified nonlinear Schrödinger model and shown that it possesses solitons in many dimensions provided that its nonlinearity is strong enough; i.e. that its coupling constant takes values larger than some critical value which depends on the dimensionality of the problem. We have also found that, in all cases, the soliton field can be well approximated by an appropriate Gaussian.

We have also proved the existence of moving solitons in our original model and have shown that the solitons can get trapped on lattice sites for slow velocities. Other, more general, configurations were found to spread out.

We are now looking at further generalizations of our model and at their possible applications.

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1. *Brizhik L., Piette B.M.A.G., Zakrzewski W.J.*//Physica. D. **146** (2000) 275—288.
2. *Brizhik L., Eremko A., Piette B.M.A.G., Zakrzewski W.J.*// Ibid. **159** (2001) 71—90.
3. *Brizhik L., Eremko A., Piette B.M.A.G., Zakrzewski W.J.* Static Solutions of a D-dimensional Modified Nonlinear Schrödinger Equation (preprint, 2002).
4. *Brizhik L., Eremko A., Piette B.M.A.G., Zakrzewski W.J.* Spontaneous Electron Localization in $2D$ Lattices. (in preparation).
5. *Hartmann B., Zakrzewski W.J.* Solitons and Deformed Lattices, I (Durham preprint, 2002).
6. *Davydov A.S., Kislukha N.I.*// Phys. status solidi. **59** (1973) 465—470.
7. *Davydov A.S.* Solitons in Molecular Systems. — Dordrecht: Reidel, 1985.
8. *Xie A., van der Meer L., Hoff W., Austin R.H.*// Phys. Rev. Lett. **84** (2000) 5435—5438.
9. *Brizhik L.S., Eremko A.A.*// Z. Phys. B. **104** (1997) 771—775.
10. *Gaididei Yu.B., Mingaleev S.F., Christiansen P.J.* //Phys. Rev. E. **62** (2000) R53—56.
11. *Mingaleev S.F., Gaididei Yu.B., Christiansen P.J., Kivshar Yu.S.*// cond-mat/0108362.
12. *Peyrard M., Bishop A.R.*//Phys. Rev. Lett. **62** (1989) 2755—2758; *Ting J.J.L., Peyrard M.*// Phys. Rev. E. **53** (1996) 1011—1020.
13. *Morse P.M.*// Phys. Rev. **34** (1929) 57—64.

СОЛІТОННІ СТАНИ ТА НЕЛІНІЙНЕ РІВНЯННЯ ШРЕДІНГЕРА В ДВОХ ТА БІЛЬШЕ ВИМІРАХ

В. Закржевські

Р е з ю м е

Наведено та обговорено деякі результати, одержані в роботах [1—4] та [5]. Показано, що для правильно вибраних значень параметрів системи, двовимірні рівняння, що описують квазічастинку, яка взаємодіє зі зміщеннями атомів гратки з їхніх рівноважних положень, мають солітонні розв'язки. Показано також, що в континуальному наближенні ефективне рівняння для квазічастинки стає нелінійним і, в загальному випадку, нелокальним рівнянням Шредінгера. Описуються умови, коли це рівняння допускає також солітонні розв'язки. Обговорюються подальші узагальнення цієї проблеми.

СОЛИТОННЫЕ СОСТОЯНИЯ И НЕЛИНЕЙНОЕ УРАВНЕНИЕ ШРЕДИНГЕРА В ДВУХ И БОЛЕЕ ИЗМЕРЕНИЯХ

В. Закржевски

Р е з ю м е

Приведены и обговариваются некоторые результаты, полученные в работах [1—5]. Показано, что при правильном выборе параметров системы двухмерные уравнения, описывающие квазичастицу, которая взаимодействует со смещениями атомов решетки из равновесных положений, имеют солитонные решения. А также показано, что в континуальном приближении эффективное уравнение для квазичастицы становится нелинейным и, в общем случае, нелокальным уравнением Шредингера. Описаны условия, при которых это уравнение также допускает солитонные решения. Обговариваются дальнейшие обобщения этой проблемы.