JHEP PROCEEDINGS

Integrable Theories, Solitons and Duality

Solitonic Electron States and the Modified Nonlinear Schrödinger Equation in 2 and More Dimensions

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ABSTRACT: We present and discus some results of [1], [2], [3] and [4]. 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 discuss the conditions when this equation also possesses solitonic solutions.

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1. INTRODUCTION

Recently, many studies have been performed [5]-[10] of organic and inorganic substances which exhibit localised modes of excitations. These modes resemble solitons. Several of these substances posses anisotropic properties, so much so that they are usually classified as low-dimensional systems (one- or two-dimensional). Some of these systems have found applications in opto- and nano-electronics, others describe biological macromolecules or synthesised biopolymers. Hence studying their properties leads not only to a better understanding of general principles but may even lead to concrete applications.

It is well understood by now that the electron-phonon interactions are very important in the dynamics of low dimensional systems and can lead to some very interesting phenomena. An example of them is a quasiparticle self-trapping which is sometimes referred to as a spontaneous or auto-localisation of a quasiparticle. Thus a comparative study of systems with similar chemical composition but belonging to classes of different dimensionalities

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would be of great interest. An example of such a system was mentioned in [10] where it was shown that the life-time of Amide-I excitation in myoglobin is much higher than the life-time of the excitations of the photoactive yellow protein.

Of course the idea of the self-trapping of Amide-I excitations in a soliton state in one-dimensional proteins has been with us for a while. This idea was, in fact, first suggested by Davydov[9, 11] already in 1975. It is also known that in effectively one dimensional system a quasi-particle (electron, hole, exciton, etc) self-trapping takes place only for a particular range of the parameters characterising the system [12]. A similar, although 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 parameters.

Generally speaking, these low-dimensional substances are characterised by the existence of a regular, often anisotropic, lattice of atoms which may deform and oscillate around their positions of equilibrium. The electrical or optical properties of these substances are governed by the collective excitations of electron states which are coupled to the oscillations of the lattice sites through an effective electron-phonon interaction. Depending on the strength of the coupling constants for these interactions the ground states of a quasiparticle can be classified as almost free quasiparticles, small polarons, or solitons. These states possess qualitatively different properties and can be derived in different approximations to the full theory.

When we look at one-dimensional systems, such as polypetides etc, we find that they possess acoustic and optical phonons and admit the existence of Davydov or molecular solitons. This derivation is based the adiabatic approximation whose validity is assumed in the derivation. In the continuum limit the collective excitations of such systems are described by a one-dimensional nonlinear Schrödinger equation with an attractive interaction. Such systems have attracted many investigations. So far, however, relatively little study has been performed of 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, 2, 3, 4].

2. HAMILTONIAN OF THE SYSTEM

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

$$\hat{H} \;=\; \hat{H}_e \;+\; \hat{H}_{ph} \;+\; \hat{H}_{int} \tag{2.1}$$

i.e. which, in the site representation, are given by:

$$\hat{H}_e = \sum_{m,n}[\mathcal{E}_0 A^+_{m,n}A_{m,n} - j_x(A^+_{m,n}A_{m+1,n} + A^+_{m+1,n}A_{m,n}) \\ -j_y(A^+_{m,n}A_{m,n+1} + A^+_{m,n+1}A_{m,n})], \tag{2.2}$$

$$\hat{H}_{ph} = \tfrac{1}{2}\sum_{m,n}\Big(\frac{\hat{p}^2_{m,n}}{M} + \frac{\hat{q}^2_{m,n}}{M} + k_x\left[(\hat{u}_{m,n}-\hat{u}_{m+1,n})^2+(\hat{v}_{m,n}-\hat{v}_{m+1,n})^2\right] + k_y\left[(\hat{u}_{m,n}-\hat{u}_{m,n+1})^2+(\hat{v}_{m,n}-\hat{v}_{m,n+1})^2\right]\Big), \tag{2.3}$$

$$\hat{H}_{int} = \sum_{m,n} A^+_{m,n}A_{m,n}\left[\chi_x(\hat{u}_{m+1,n}-\hat{u}_{m-1,n})+\chi_y(\hat{v}_{m,n+1}-\hat{v}_{m,n-1})\right]. \tag{2.4}$$

In these expressions $A^+_{m,n}$ ($A_{m,n}$) denote the creation (annihilation) operators of the electron on 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; j_x, j_y are the exchange interaction energies, and 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.

$\hat{H}_{int}$, the Hamiltonian of the interaction, is taken in the simplest form [11] and so it only involves the "nearest neighbour" interaction between the electron field and the deformation of the lattice. Later, we shall discuss generalisations of this assumption.

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

Thus our Hamiltonian becomes

$$H = \sum_{m,n}\Big((\mathcal{E}_\prime + \mathcal{W})\,|\varphi_{m,n}|^2 - j_x\,\varphi^*_{m,n}(\varphi_{m+1,n}+\varphi_{m-1,n}) - j_y\,\varphi^*_{m,n}(\varphi_{m,n+1}+\varphi_{m,n-1}) + |\varphi_{m,n}|^2[b\chi_x\,(u_{m+1,n}-u_{m-1,n}) + a\chi_y\,(v_{m,n+1}-v_{m,-1})], \tag{2.5}$$

where W describes the phonon energy and is given by

$$\mathcal{W} = \tfrac{1}{2}\sum_{m,n}\Big(\frac{p^2_{m,n}}{M} + \frac{q^2_{m,n}}{M} + k_x\left[(u_{m,n}-u_{m+1,n})^2+(v_{m,n}-v_{m+1,n})^2\right] + k_y\left[(u_{m,n}-u_{m,n+1})^2+(v_{m,n}-v_{m,n+1})^2\right]\Big). \tag{2.6}$$

Let us note that we have a constraint: the electron wave function must satisfy the normalisation condition

$$\sum_{m,n}|\varphi_{m,n}|^2 = 1. \tag{2.7}$$

This normalisation condition is less important in one dimension for one extra electron. However, such a normalisation condition 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 extra electron.

Next, to simplify our expressions we introduce dimensionless units:

$$\tau = \frac{j_x t}{\hbar}, \quad U = C_x \frac{u}{b}, \quad V = C_x \frac{v}{b}, \quad E_s = \frac{b^2 M j_x}{\hbar^2}, \quad E_0 = \frac{\mathcal{E}_\prime}{j_x},$$
$$C_x = \frac{\chi_x b^2}{j_x}, \quad C_y = \frac{\chi_y a b}{j_x}, \quad K_x = \frac{k_x \hbar^2}{M j_x^2}, \quad K_y = \frac{k_y \hbar^2}{M j_x^2}, \quad g = \frac{2 C_x^2}{K_x E_s} \tag{2.8}$$

and also the anisotropy parameters:

$$A_j = \frac{j_y}{j_x}, \qquad A_c = \frac{C_y}{C_x}, \qquad A_k = \frac{K_y}{K_x}. \tag{2.9}$$

It is easy to derive the Euler- Lagrange equations describing our system. They are given by:

$$i \frac{d\varphi_{m,n}}{d\tau} = (E_0 + W)\varphi_{m,n} - (\varphi_{m+1,n} + \varphi_{m-1,n}) - A_j (\varphi_{m,n+1} + \varphi_{m,n-1}) + [(U_{m+1,n} - U_{m-1,n}) + A_c (V_{m,n+1} - V_{m,n-1})]\varphi_{m,n}, \tag{2.10}$$

$$\frac{d^2 U_{m,n}}{d\tau^2} = -\frac{K_x}{C_x}[(2U_{m,n} - U_{m+1,n} - U_{m-1,n}) + A_k (2U_{m,n} - U_{m,n+1} - U_{m,n-1}) - \frac{g}{2}(|\varphi_{m+1,n}|^2 - |\varphi_{m-1,n}|^2)], \tag{2.11}$$

$$\frac{d^2 V_{m,n}}{d\tau^2} = -\frac{K_x}{C_x}[(2V_{m,n} - V_{m+1,n} - V_{m-1,n}) + A_k (2V_{m,n} - V_{m,n+1} - V_{m,n-1}) - \frac{g A_c}{2}(|\varphi_{m,n+1}|^2 - |\varphi_{m,n-1}|^2)], \tag{2.12}$$

with the phonon energy given by:

$$W = \tfrac{1}{2} E_s \sum_{m,n} \Big(P_{m,n}^2 + Q_{m,n}^2 + \frac{K_x}{C_x}([(U_{m,n} - U_{m+1,n})^2 + (V_{m,n} - V_{m+1,n})^2] + A_k[(U_{m,n} - U_{m,n+1})^2 + (V_{m,n} - V_{m,n+1})^2]) \Big), \tag{2.13}$$

where

$$P_{m,n} = \frac{dU_{m,n}}{d\tau}, \quad Q_{m,n} = \frac{dV_{m,n}}{d\tau}. \tag{2.14}$$

3. STATIONARY CASE

To proceed further we, first of all, consider the stationary case. Then the equations (2.10-2.12) reduce to

$$\lambda \varphi_{m,n} + (2\varphi_{m,n} - \varphi_{m+1,n} - \varphi_{m-1,n}) + A_j (2\varphi_{m,n} - \varphi_{m,n+1} - \varphi_{m,n-1}) + [(U_{m+1,n} - U_{m-1,n}) + A_c (V_{m,n+1} - V_{m,n-1})]\varphi_{m,n} = 0, \tag{3.1}$$

$$(2U_{m,n} - U_{m+1,n} - U_{m-1,n}) + A_k (2U_{m,n} - U_{m,n+1} - U_{m,n-1}) = \frac{g}{2}(|\varphi_{m+1,n}|^2 - |\varphi_{m-1,n}|^2), \tag{3.2}$$

$$(2V_{m,n} - V_{m+1,n} - V_{m-1,n}) + A_k (2V_{m,n} - V_{m,n+1} - V_{m,n-1}) = \frac{g A_c}{2}(|\varphi_{m,n+1}|^2 - |\varphi_{m,n-1}|^2), \tag{3.3}$$

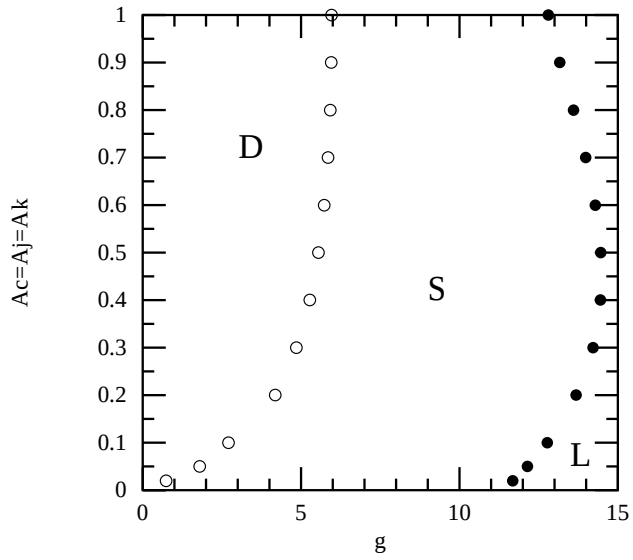

Figure 1: A typical phase diagram for the case $A_j = A_k = A_c$

where $\lambda = E_0 + W - 2(1 + A_j)$.

We have analysed these equations, numerically, for various choices of parameters. The results are presented in [1] and [2]. The phase diagrams given in [1] clearly exhibit the role of the anisotropy. In Figure 1 we exhibit the range of parameters for which we have a solution of the equations as a function of g and of the common anisotropy parameter $A = A_j = A_k = A_c$. The solitons exist in the middle region marked "S" in Figure 1. The region "D" corresponds to the "almost free" (delocalised) electrons while the region "L" is the region of extremely localised solitons - "small polarons" (essentially localised to one lattice point).

In Figure 2 we present the plots of $|\varphi|$, and of $U = V$ for the case corresponding to $g = 6.8$ and to the isotropic condition (i.e. $A_j = A_k = A_c = 1$).

In the rest of this talk we restrict our attention to the isotropic case. Further results on the anisotropic cases can be found in [1].

4. ISOTROPIC CASE

In the isotropic system we have $A_j = A_k = A_c = 1$. Next we define

$$\Delta(1)U_{m,n} = 4U_{m,n} - U_{m+1,n} - U_{m-1,n} - U_{m,n+1} - U_{m,n-1}, \tag{4.1}$$

and

$$\Delta(2)|\varphi_{m,n}|^2 = 4|\varphi_{m,n}|^2 - |\varphi_{m+2,n}|^2 - |\varphi_{m-2,n}|^2 - |\varphi_{m,n+2}|^2 - |\varphi_{m,n-2}|^2. \tag{4.2}$$

Noting that, as $A_k = 1$, (3.2) and (3.3) can be written as

$$\Delta(1)(U_{m+1,n} - U_{m-1,n}) = \tfrac{g}{2}(|\varphi_{m+2,n}|^2 - |\varphi_{m,n}|^2 - |\varphi_{m,n}|^2 + |\varphi_{m-2,n}|^2) \tag{4.3}$$

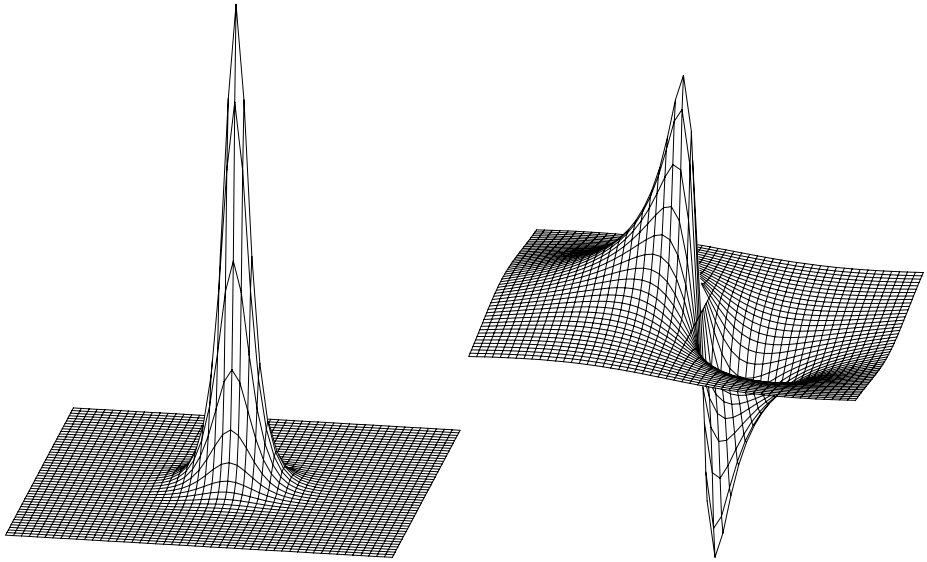

Figure 2: Soliton for $g = 6.8$. Left: $|\varphi|$; Right: U

$$\Delta(1)(V_{m,n+1} - V_{m,n-1}) = \tfrac{g}{2}(|\varphi_{m,n+2}|^2 - |\varphi_{m,n}|^2 - |\varphi_{m,n}|^2 + |\varphi_{m,n-2}|^2), \qquad (4.4)$$

we see that

$$\Delta(1)\left((U_{m+1,n} - U_{m-1,n}) + (V_{m,n+1} - V_{m,n-1})\right) = -\tfrac{g}{2}\Delta(2)|\varphi_{m,n}|^2. \qquad (4.5)$$

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

$$\Delta(1)Z_{m,n} = -\tfrac{g}{2}\Delta(2)|\varphi_{m,n}|^2, \qquad (4.6)$$

where

$$Z_{m,n} = (U_{m+1,n} - U_{m-1,n}) + (V_{m,n+1} - V_{m,n-1}). \qquad (4.7)$$

In (4.6) $\Delta(1)$ describes a 5 point Laplacian and $\Delta(2)$ is the same operator but, effectively, missing out the nearest points of the lattice (*ie* an operator on a lattice twice as large). 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

$$P_{i+1} + P_{i-1} - 2P_i = \kappa(2R_i - R_{i+2} - R_{i-2}). \qquad (4.8)$$

is solved by

$$P_n = -\kappa(R_{n+1} + R_{n-1} + 2R_n) \qquad (4.9)$$

where we have neglecyted the boundary terms. Equation (4.6) will, nevertheless, be useful later on.

5. CONTINUUM LIMIT

Next we look at the continuum limit of our equations (3.1-3.3). To do this 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

$$\varphi_{m\pm1,n} = \varphi_{m,n} \pm \frac{\partial\varphi(x,y)}{\partial x} + \frac{1}{2}\frac{\partial^2\varphi(x,y)}{\partial x^2} \pm \frac{1}{6}\frac{\partial^3\varphi(x,y)}{\partial x^3} + \frac{1}{24}\frac{\partial^4\varphi(x,y)}{\partial x^4} + \dots \tag{5.1}$$

$$U_{m\pm1,n} = U_{m,n} \pm \frac{\partial U}{\partial x} + \frac{1}{2}\frac{\partial^2 U}{\partial x^2} \pm \frac{1}{6}\frac{\partial^3 U}{\partial x^3} + \frac{1}{24}\frac{\partial^4 U}{\partial x^4} + \dots \tag{5.2}$$

$$V_{m,n\pm1} = V_{m,n} \pm \frac{\partial V}{\partial y} + \frac{1}{2}\frac{\partial^2 V}{\partial x^2} \pm \frac{1}{6}\frac{\partial^3 V}{\partial x^3} + \frac{1}{24}\frac{\partial^4 V}{\partial x^4} + \dots \tag{5.3}$$

we can write

$$\frac{\partial^2 U}{\partial x^2} = -g\left(\frac{\partial|\varphi|^2}{\partial x} + \frac{1}{6}\frac{\partial^3}{\partial x^3}|\varphi|^2\right) \tag{5.4}$$

$$\frac{\partial^2 V}{\partial x^2} = -g\left(\frac{\partial|\varphi|^2}{\partial y} + \frac{1}{6}\frac{\partial^3}{\partial y^3}|\varphi|^2\right), \tag{5.5}$$

where we have neglected $\frac{\partial^2 U}{\partial y^2}$ and $\frac{\partial^2 V}{\partial x^2}$. Integrating (30) and (31) and setting all "constants of integration" to zero we get

$$\frac{\partial U}{\partial x} = -g\left(|\varphi|^2 + \frac{1}{6}\frac{\partial^2}{\partial x^2}|\varphi|^2\right) \tag{5.6}$$

$$\frac{\partial V}{\partial y} = -g\left(|\varphi|^2 + \frac{1}{6}\frac{\partial^2}{\partial y^2}|\varphi|^2\right) \tag{5.7}$$

and so the φ equation becomes:

$$i\frac{d\varphi}{d\tau} + \Delta\varphi + 2g\left(|\varphi|^2 + \frac{1}{12}\Delta|\varphi|^2\right)\varphi = 0, \tag{5.8}$$

ie a **Nonlinear Schrödinger Equation** but with an extra term.

This equation, without the extra term, has been studied before. It is well known that, in one dimension, it possesses a soliton solution for an arbitrary value of g. In two dimensions, however, the soliton solution is stable only if our extra term is present.

6. EXISTENCE OF SOLITONS

Next we present some arguments from [3] which allows us to "understand" our numerical results. Thus we consider two limits of our equations, when we can perform some approximations; namely, we consider the broad solitons and the narrow solitons.

6.1 Broad solitons

Let us look first at the broad solitons. In this case we expect the continuum limit approximation to be valid and so we base our discussion on our Nonlinear Schrödinger Equation (5.8). This equation, clearly, possesses a conserved energy which is given by:

$$\mathcal{E} = \int\left[|\vec{\nabla}\varphi|^2 - g|\varphi|^4 + \frac{g}{12}\left(\Delta|\varphi|^2\right)^2\right]dxdy. \tag{6.1}$$

Clearly, had we neglected the last term in (5.8) and so used only the Schrödinger equation

$$i\frac{d\varphi}{d\tau} + \Delta\varphi + 2g|\varphi|^2\varphi = 0 \tag{6.2}$$

its solutions would have been unstable but, we have this extra term which comes from the lattice and it has stabilised the solitons. To get a better understanding of this effect we consider first the square of the size of any localised, soliton-like, configuration

$$R^2 = \int |\varphi(x,y)|^2 (x^2+y^2) dxdy. \tag{6.3}$$

Differentiating with respect to τ and using (5.8) we get:

$$\tfrac{dR^2}{d\tau} = -\int (x^2+y^2)(\varphi\Delta\varphi^* - \varphi^*\Delta\varphi) dxdy. \tag{6.4}$$

and so we see that

$$\tfrac{d^2R^2}{d\tau^2} = 8(\mathcal{E}+\delta), \tag{6.5}$$

where

$$\delta = \tfrac{g}{12}\int \left(\Delta|\varphi|^2\right)^2 dxdy. \tag{6.6}$$

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 stabilisation of the soliton.

To get a better "feeling" for this let us consider the example of a Gaussian wave function (which, in fact, is not a bad approximation for a soliton). Thus we consider

$$\varphi(x,y) = \frac{\kappa}{\sqrt{\pi}}\, exp\left(-\frac{\kappa^2}{2}(x^2+y^2)\right). \tag{6.7}$$

and then insert it into (6.1). We find that

$$\mathcal{E} = \kappa^2(1-\frac{g}{2\pi}) + g\frac{\kappa^4}{12\pi} \tag{6.8}$$

and so we see that the value of κ minimising $\mathcal{E}$ is given by

$$\kappa_0^2 = 3(1-\frac{2\pi}{g}). \tag{6.9}$$

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 (3.1-3.3) numerically we have found $g_{cr} \approx 5.85$, which is clearly not so different from 2π. The above-mentioned interplay between the shrinking and expanding of the solitons can also be studied in this example. The results are given in [1].

6.2 Narrow solitons

Next we look at the narrow solitons. Based on the experience gained by performing numerical simulations we assume that the solitons are restricted to a very few lattice points. This is meant to be true not only for the φ field but also for U and V fields (although they are less localised than the field φ).

To do this we look at the eigenvalue equation for φ

$$-\lambda\varphi_{m,n} = -(\varphi_{m+1,n}+\varphi_{m-1,n}+\varphi_{m,n+1}+\varphi_{m,n-1}-4\varphi_{m,n}) + Z_{m,n}\varphi_{m,n}, \tag{6.10}$$

where $Z_{m,n}$ defined by (4.7) satisfies (4.6).

As we cannot solve (6.10) exactly we attempt to solve it iteratively. Thus, first we assume that $|\varphi_{0,0}|^2 = 1$ and all other $|\varphi_{m,n}|^2$ zero. We find

$$Z_{0,0} = -\tfrac{8}{11}g, \qquad Z_{1,0} = -\tfrac{5}{22}g, \qquad Z_{1,1} = -\tfrac{4}{33}g, \qquad Z_{2,0} = \tfrac{2}{33}g, \qquad Z_{2,1} = -\tfrac{1}{66}g. \tag{6.11}$$

Then we use this result to determine a "new-modified" φ. So we assume

$$\begin{aligned} \varphi_{0,0} &= 1 - \tfrac{F}{g^2}, \\ \varphi_{m,n} &= f_{m,n}\, g^{-(|m|+|n|)}. \end{aligned} \tag{6.12}$$

Moreover, we impose

$$f_{m,n} = f_{|m|,|n|}. \tag{6.13}$$

Then we find

$$\begin{aligned} \lambda &= -4 + \tfrac{8}{11}g, \qquad f_{1,0} = 2 \\ f_{1,1} &= \tfrac{33}{5}, \qquad f_{2,0} = \tfrac{33}{13}, \qquad F = 8 \end{aligned} \tag{6.14}$$

which is, in fact, in good agreement with the solutions determined numerically! In Figure 3 we show $(4+\lambda)/g$, $f_{1,0} = g\varphi_{1,0}$ and $F = g^2(1-\varphi_{0,0})$ determined numerically. We see that our results are in fact, valid for a suprisingly large range of g, and not only in the limit $g \to \infty$.

7. OTHER (BETTER) APPROXIMATIONS

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

(i) a Gaussian function

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

(ii) a decreasing exponent

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

and (iii) a hyperbolic secant

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

where $A_i, i = 1,2,3$ are normalisation coefficients.

They have all produced qualitatively similar results as has been discussed in [2].

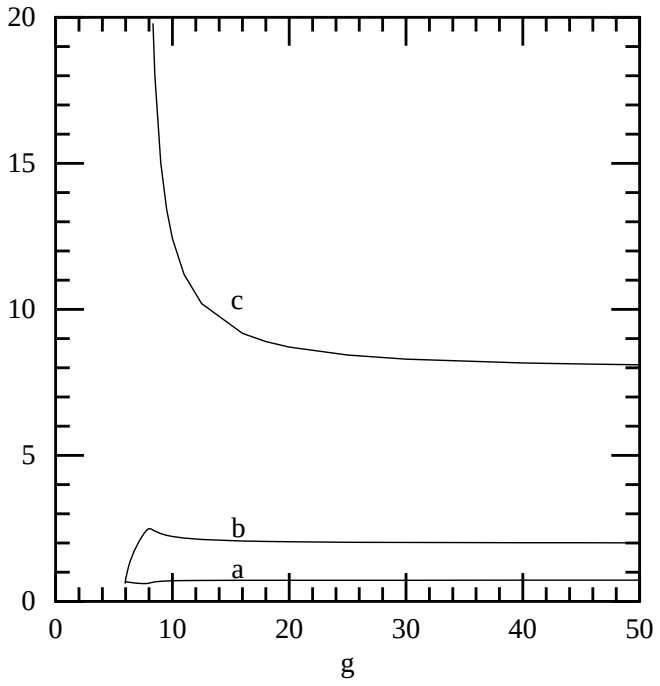

Figure 3: Numerically determined g dependence of (a) the energy $(4+\lambda)/g$ (b) $f_{1,0} = g\varphi_{1,0}$ and (c) $F = g^2(1-\varphi_{0,0})$,

A better approximation involves the use of the elliptic functions; namely, we can put

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

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

In Figure 4 we present the plot of $\frac{1}{R}$ as a function of g as given in [2]. We see that the gaussian ansatz gives a very good approximation when $g < 8$. The elliptic function approximation, shown in Figure 4b, is the only ansatz that has managed to reproduce the "shoulder" appearing in the numerically determined curve, but it is nevertheless less accurate than the gaussian ansatz for small values of g.

8. MOVING SOLITONS

We have also studied moving solitons. To do this we 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 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 shape) except in some cases of essentially

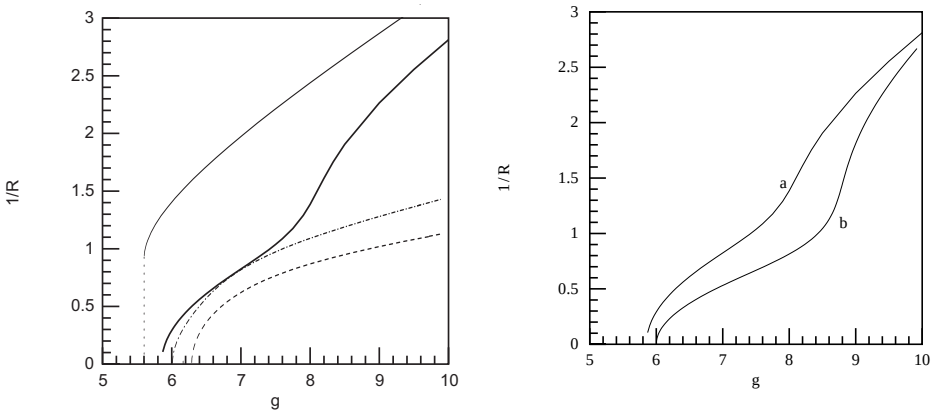

Figure 4: Inverse width of the localisation region, $1/R(g)$, for different trial functions: Left: solid line: decreasing exponent; dashed line: gaussian; dot-dashed: hyperbolic secant. thick solid line: numerical evaluation. Right : a) numerical evaluation b) elliptic function approximation

"head-on" collisions. 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 physicial as they describe interactions of chargeless states.

9. MODIFIED NLSE in D DIMENSIONS

Given the relevance of our modified NLSE we have decided to study it in more detail. Here we reproduce some of the results of [3] where we consider the problem, in general, in D dimensions. Thus we study the equation

$$i\varphi_t + \Delta\varphi + 2\left(g|\varphi|^2 + G\Delta|\varphi|^2\right)\varphi = 0. \tag{9.1}$$

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

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

1. The norm functional
$$N = \int dx^D |\varphi|^2, \tag{9.2}$$

2. Energy
$$H = \int dx^D \left(|\vec{\partial}\varphi|^2 - g|\varphi|^4 + G(\vec{\partial}|\varphi|^2)^2\right) \tag{9.3}$$

3. Momentum
$$\vec{I} = \int dx^D \vec{j}, \qquad j_\mu = -\tfrac{i}{2}\left(\varphi^* \tfrac{\partial\varphi}{\partial x_\mu} - \varphi\tfrac{\partial\varphi^*}{\partial x_\mu}\right) \tag{9.4}$$

and

4. Angular momentum
$$L_{\mu\nu} = \int dx^D \left(x_\mu j_\nu - x_\nu j_\mu\right). \tag{9.5}$$

D	Numerical g_{cr}	Ansatz g_{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	$5(\pi)^{5/2}(35/18)^{3/2} \approx 237.16$

Table 1: Critical values g_{cr} determined numerically and by the Gaussian ansatz.

It is convenient to define also the **eigen-energy**

$$\Lambda = \int dx^D \tfrac{i}{2} \left(\varphi^* \tfrac{\partial \varphi}{\partial t} - \varphi \tfrac{\partial \varphi^*}{\partial t} \right). \tag{9.6}$$

Then for a solution of the form (stationary solution)

$$\varphi = \phi e^{-i\lambda t} \tag{9.7}$$

we find that

$$\Lambda = \lambda N. \tag{9.8}$$

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

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

- The equation has solitonic solutions for $g > g_{cr}$.
- g_{cr} depends on D (dimension).
- g_{cr} grows with the increase of D.

In Table 1 we present our results on the value of g_{cr} determined numerically and determined by the Gaussian ansatz. As we see the agreement betwen the two expressions is amazingly good.

Many 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).
- 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_{cr} also increases with the value of l.
- Soliton can be made to move - so we can study their dynamics.

In Figure 5. we present the energy H/λ for various values of g. We notice that for $D > 2$ there exist two solutions for some values of g but that the second solution has a positive energy and is thus unstable.

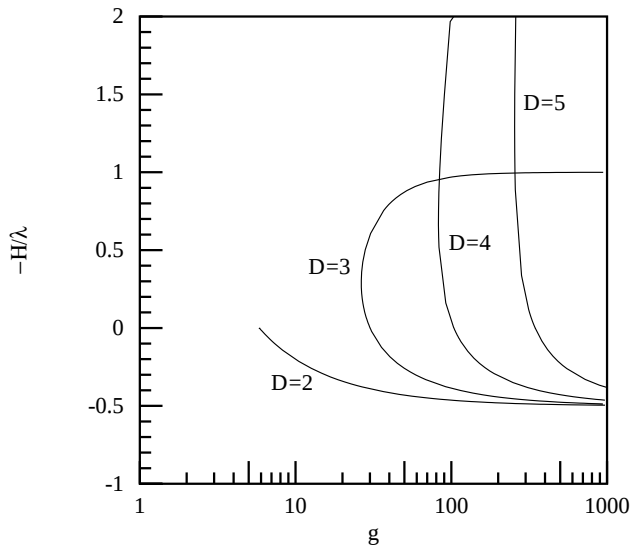

Figure 5: H/λ as a function of g for D=2 to 5

10. MORE GENERAL INTERACTIONS

Finally, we return to our original problem discussed in section 2. There, in the one dimensional case, we considered the interaction Hamiltonian given by:

$$\hat{H}_{int} = \chi \sum_i A_i^\dagger A_i \, (\hat{U}_{i+1} - \hat{U}_{i-1}). \tag{10.1}$$

Let us now generalise this further by considering

$$\hat{H}_{int} = \sum_{ij} A_i^\dagger A_i \, K_{ij} \hat{U}_j, \tag{10.2}$$

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

$$\hat{H} = \sum_m \left[\frac{P_m^2}{2M} + \kappa (U_m - U_{m+1})^2 - \sum_l J_{lm} \phi_m^\dagger \phi_l + c.c + \sum_k K_{mk} |\phi_m|^2 U_k \right], \tag{10.3}$$

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:

$$i \frac{d\phi_m}{dt} = E\phi_m - \sum_l J_{lm} \phi_l - \sum_k K_{mk} \phi_m U_k \tag{10.4}$$

and

$$\frac{d^2U_m}{dt^2} \,=\, \kappa(2U_m - U_{m+1} - U_{m-1}) \,+\, \sum_k K_{km}|\phi_k|^2. \tag{10.5}$$

The second equation is really the spatially discretised version of

$$\Box U_m \,=\, P_m \tag{10.6}$$

and so has a solution:

$$U_m \,=\, \sum_n G_{mn}\, P_n, \tag{10.7}$$

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

Thus we see that

$$U_m \,=\, \sum_{nk} G_{mn}\, K_{kn}\, |\phi_k|^2 \,=\, \sum_k \tilde{G}_{mk}\, |\phi_k|^2 \tag{10.8}$$

and so, after some redefinitions,

$$i\frac{d\phi_m}{dt} \,=\, E\phi_m - \sum_l J_{lm}\phi_l - \sum_k K_{mk}\phi_m \sum_l \tilde{G}_{kl}|\phi_l|^2 = E\phi_m - \sum_l J_{lm}\phi_l - \sum_r Z_{mr}\,\phi_m|\phi_r|^2. \tag{10.9}$$

Note that the last term in our ϕ equation comes from

$$V(|\phi|^2) \,=\, \sum_{mr} Z_{mr}\, |\phi_m|^2\, |\phi_r|^2, \tag{10.10}$$

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

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

Let us note that:

- this discussion generalises to higher dimensions,
- we can present a different derivation based on the original equations,
- other interesting systems have been studied (like systems on a chain which can deform itself).

11. CONCLUSIONS and GENERAL COMMENTS

We have given an overview of our recent results [1-4]. 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

more general case, leads to a nonlocal version of this model. The details of the nonlocality depend on the coupling between the electron field and the deformations of the lattice.

The nonlocality, in the specific cases studied by us, is responsible for the existence of solitons. We have also analysed our modified nonlinear Schrödinger model and showed that it possesses solitons in many dimensions provided that its nonlinearity is strong enough; ie that its coupling constant takes values larger than some critical value (which increases as we increase the spatial dimension). We have also found that, in all cases, the soliton field is approximated well by an appropriate Gaussian.

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

We are also looking at futher generalisations of our models and results and at their possible applications.

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