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The Transition of 2-Dimensional Solitons to 1-Dimensional Ones on Hexagonal Lattices

Betti HARTMANN [a] *and Wojtek J ZAKRZEWSKI* [b]

[a] *School of Engineering and Sciences, International University Bremen (IUB)*
28725 Bremen, Germany
E-mail: b.hartmann@iu-bremen.de

[b] *Department of Mathematical Sciences, University of Durham*
Durham DH1 3LE, UK
E-mail: w.j.zakrzewski@durham.ac.uk

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Abstract

We study solitons arising in a system describing the interaction of a two-dimensional discrete hexagonal lattice with an additional electron field (or, in general, an exciton field). We assume that this interaction is electron-phonon-like. In our previous paper [4] we have studied the existence of two-dimensional solitons and have found that these solitons exist only if the electron-phonon coupling constant is sufficiently large. In this paper, we report the results of our investigation for small values of this constant, close to its critical value for the existence of solitons. We find that as the coupling decreases the soliton gets very broad and then becomes effectively one-dimensional.

1 Introduction

Recently, a Fröhlich Hamiltonian was studied on a two-dimensional, discrete, quadratic [1, 2, 3], respectively hexagonal lattice [4]. It is well known that the interaction of an excitation field such as an amide I- vibration in biopolymers or an electron (in the case of the Fröhlich Hamiltonian) with a lattice whose distortion can be caused by this excitation results in the creation of a localised state which, in what follows, we refer to as a soliton. Such a soliton was first introduced by Davydov [5] in the 1970s to explain the dispersion free energy transport in biopolymers (see also [6] for further details). In [1, 2, 4], the existence of such solitons was studied numerically and it was found that their properties depended crucially on the magnitude of the electron-phonon coupling constant. In particular, localised 2-dimensional structures exist only above a critical value of this coupling. These numerical results have been confirmed by a simple analytic argument: using a Gaussian in 2 dimensions, we can approximate very well this critical value.

In this paper, we extend the results for the soliton on a hexagonal lattice [4] and look at the properties of the solitons close to the critical coupling. We find that close to this critical coupling, three types of solutions exist: the "narrow" 2-dimensional solitons, discussed in

[4], "broad" 2-dimensional solitons, which extend over much bigger parts of the lattice than the former, and one-dimensional solitons. Since our model is a toy-model for solitons on nanotubes, these latter configuartions can be interpreted as ring-like solitonic structures around the tube.

In section II we present our equations and in section III we discuss the results of our numerical investigations.

2 Basic Equations

The equations describing an electron field interacting with a deformable hexagonal lattice were derived in [4]. These equations read:

$$
\begin{aligned}
i\frac{\partial\psi_{i,j}}{\partial\tau} &= (E_0+W_0)\psi_{i,j} - 2\left(\psi_{i+1,j+1}+\psi_{i-1,j}+\psi_{i+1,j-1}\right) \\
&+ \psi_{i,j}\left[(U_{i+1,j+1}+U_{i+1,j-1}-2U_{i-1,j})+\sqrt{3}(V_{i+1,j+1}-V_{i+1,j-1})\right] , \qquad (2.1)
\end{aligned}
$$

for the electron field and

$$
\begin{aligned}
\frac{d^2U_{i,j}}{d\tau^2} &= K_x\left(3U_{i,j}-U_{i+1,j+1}-U_{i-1,j}-U_{i+1,j-1}\right) \\
&+ \frac{g}{2}\left(2|\psi_{i-1,j}|^2-|\psi_{i+1,j+1}|^2-|\psi_{i+1,j-1}|^2\right) , \qquad (2.2)
\end{aligned}
$$

$$
\begin{aligned}
\frac{d^2V_{i,j}}{d\tau^2} &= K_x\left(3V_{i,j}-V_{i+1,j+1}-V_{i-1,j}-V_{i+1,j-1}\right) \\
&- \frac{\sqrt{3}g}{2}\left(|\psi_{i+1,j+1}|^2-|\psi_{i+1,j-1}|^2\right) \qquad (2.3)
\end{aligned}
$$

for the displacement fields U and V in the x- and, respectively, y-direction. i and j index the points in x-, respectively y-directions.

For the corresponding Hamiltonian and the appropriate rescalings, we refer the reader to [4]. Note that K_x is the self-coupling constant of the displacement fields and g is the electron-phonon coupling. W_0 is the phonon energy, while E_0 was chosen to be 0.142312 in our numerical investigations. We have normalised the electron-function ψ to one, i.e. $\sum_{i,j=1}^{N_x,N_y}\psi_{i,j}\psi^*_{i,j}=1$ thus assuming the excitation to be one excess electron. Note that N_x and N_y denote the number of lattice points in x-, respectively y-directions.

3 Numerical results

In this paper, we present new results on a model describing the interaction of one excess electron with a 2-dimensional hexagonal lattice. This model was studied first in [4]. Before we discuss our new results, let us summarize the results of [4]. In [4] it was found that 2-dimensional solitonic structures which are created due to the interaction between the distortions of the hexagonal lattice ("phonons") and the electron field on this lattice ("excess electron"), exist only when the electron-phonon coupling is large enough. This numerical result was also found in the case of the quadratic lattice [1, 3, 2] and thus seems to be a generic feature of 2-dimensional lattices. For values of the coupling constant smaller than some critical value g_{cr}, the interaction between the lattice and the electron (exciton) field becomes too small for 2-dimensional solitonic structures to exist. In this paper, we present new results on the behaviour of the system close to this critical value g_{cr}. We have confirmed that "narrow", i.e. well pronounced 2-dimensional solitons exist for $g > 2.296$. A typical solution of this type is shown in Fig. 1 for $N_x = 160$ and $N_y = 20$.

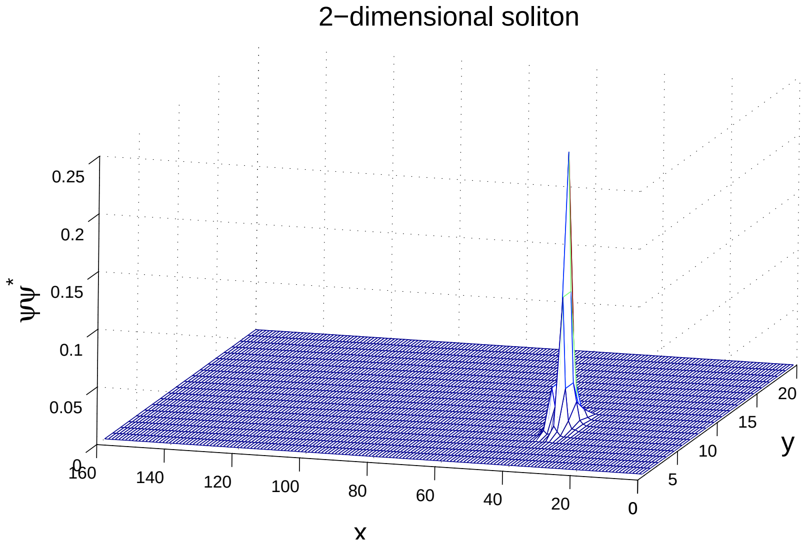

Figure 1. A typical "narrow" 2-dimensional solitonic structure on a $N_x \times N_y = 160 \times 20$ lattice for g close to the critical value $g_{cr} = 2.296$.

Clearly the probability density $\psi\psi^*$ is localised only on a small portion of the lattice. For $g \, \epsilon \, [2.29475 : 2.32592]$, a broad two-dimensional soliton appears (see Fig.3), while decreasing the value of g further leads to a configuration in which the soliton becomes effectively one-dimensional. A typical one-dimensional configuration is shown in Fig.2.

As is obvious from this figure, for small g, the function $\psi_{i,j}$ becomes effectively independent of the y-direction and we see N_y copies of the function ψ_i. While for $g \to \infty$, we expect the solitonic structure to be effectively fixed to one point on the lattice, thus $(\psi_{i,j}\psi^*_{i,j})_{max} =: (\psi\psi^*)_{max} \to 1$, the threshold of our one-dimensional soliton is characterised by the value of $(\psi\psi^*)_{max}$, which can be obtained for the last possible "broad" soliton divided by the number N_y. In our case $N_y = 20$ and the last value of the broad soliton $(\psi\psi^*)_{max} \approx 2.84 \cdot 10^{-2}$, so we would expect solitons with heights on the order of $1.42 \cdot 10^{-3}$. Indeed, for $g < 2.29475$, we find solitons with heights of $\approx 1.62 \cdot 10^{-3}$, which confirms our interpretation. We plot the g dependence of the value of $(\psi\psi^*)_{max}$ in Fig.3. Clearly, we note the familiar structure of the curve, especially, we notice that at $g \approx 1.0$, the value of $(\psi\psi^*)_{max}$ becomes constant and is equal to $(\psi\psi^*)_{max} = 3.125 \cdot 10^{-4}$. This is not surprising since this is just the value where $\psi\psi^* = 1/(N_x N_y) = 1/(160 \cdot 20) \approx 3.125 \cdot 10^{-4}$, i.e. the field is completely delocalised, i.e. it is equally distributed over the whole grid.

The fact that the one-soliton ceases to exist is, however, related to the number N_y. In principle, one-d solitons should exist for all values of $2.29475 \geq g \geq 0$. Of course, this value was derived for $\sum_{i,j} \psi_{i,j}\psi^*_{i,j} = 1$. To study the dependence on N_y, we have looked

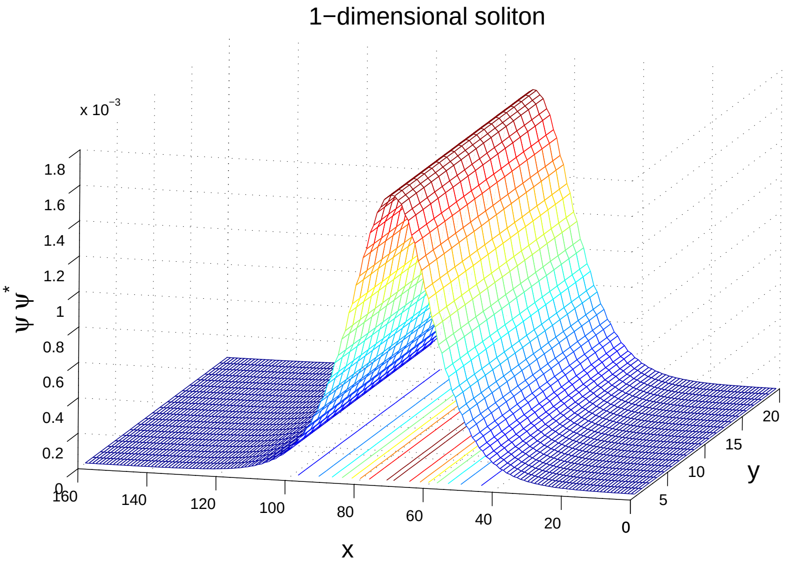

Figure 2. A typical one-dimensional solitonic structure on a $N_x \times N_y = 160 \times 20$ lattice for $g = 2.295$.

at the dependence of the critical value of g, $g_{cr,1d}(N_y)$ at which the one-d soliton becomes equally distributed over the grid, i.e. $\psi_{i,j}\psi^*_{i,j} = 1/(N_x N_y)$. The values are listed in Table I.

Table I: Dependence of $g_{cr,1d}$ on N_y for $N_x = 160$

N_y	N_y^{-1}	$g_{cr,1d}(N_y)$
20	0.050	1.00
16	0.062	0.88
12	0.083	0.67
6	0.167	0.30

We notice that the value $g_{cr,1d}(N_y)$ decreases with increasing N_y^{-1}. Since N_y^{-1} represents the normalisation of the electron field function in the x-direction, i.e. of the one-d soliton for one fixed y, this means that the "bigger" the one-d soliton is the lower is the critical value of the electron-phonon coupling. We can understand this behaviour by observing that by scaling the ψ field in our equations (2.1)-(2.3) such that $\psi_{i,j}\psi^*_{i,j} \rightarrow N_y^{-1}(\psi_{i,j}\psi^*_{i,j})$ we obtain the equations for a system with a normalization of the ψ fields corresponding to the one-d solitons. We notice that this rescaling is nothing else but the rescaling of the coupling constant $g \rightarrow N_y^{-1} g$. Following this argument, the product $N_y^{-1} g_{cr,1d}$ should thus be constant. Looking at Table I, we indeed find that $N_y^{-1} g_{cr,1d} \approx 0.05$.

We have also plotted the corresponding energies of the solutions. These are shown in Fig.4. Note that the configurations with equally distributed ψ would have an energy ≈ -5.8576. The energies of the soliton solutions are clearly below this value. The energy of a narrow soliton is the lowest energy configuration as long as the coupling constant is

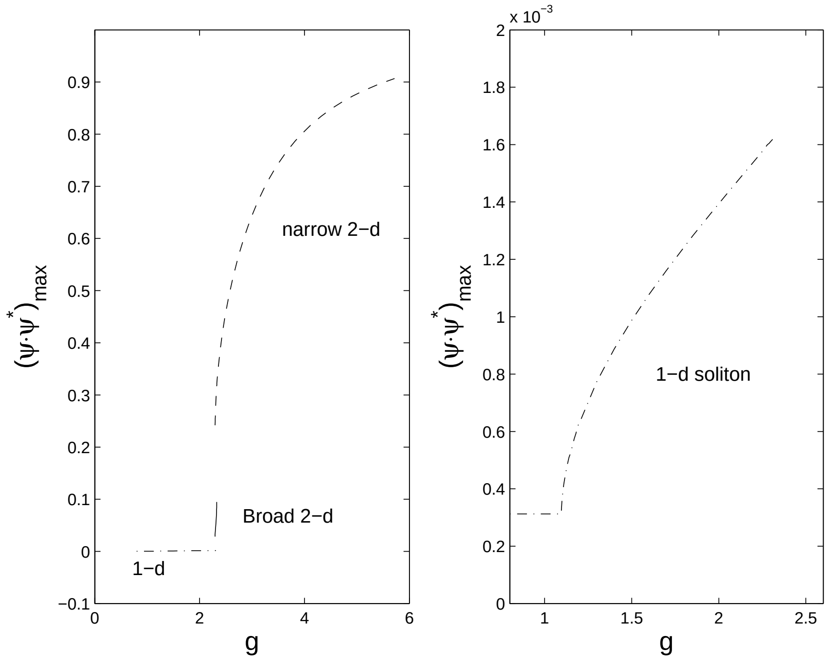

Figure 3. The g dependence of the height $(\psi\psi^*)_{max}$ of the two-dimensional and one-dimensional solitons. Note that there exist "narrow" (dashed line) and "broad" (solid line) two-dimensional solitons. The figure on the right presents the zoom of the one-d soliton curve (dotted-dashed).

above the value at which one-d solitons can exist. Then, these one-d solitons have the lowest energy. Note that the broad soliton never becomes the lowest energy configuration and so appears to be unstable.

4 Conclusions

In this short note we have reported results of our studies of an electron phonon system on a hexagonal lattice which was longer in one direction than the other (i.e. with a larger number of lattice points in the x-direction - N_x than in the y-direction i.e. N_y). We have looked at the values of the electron-phonon coupling constant at which the system possesses soliton-like solutions. We have found that "genuine" two-dimensional solitons, like those studied in [4], exist for the coupling constant larger than some critical value. For the values of the constant close to this critical value the system possesses another solution - which corresponds to a "broad" soliton. This new solution appears to be unstable. When the coupling constant is below its critical value the two-dimensional soliton is so "broad" that it can be interpreted as an effective one-dimensional structure. As the value of the coupling decreases further the "one-dimensional" soliton becomes broader and, below some new critical value, it spreads over the whole lattice leading to complete delocalisation.

The value at which this happens depends on the size of the lattice. However, this is not surprising as for an effective one-dimensional soliton the normalisation of the electron field plays an important role (the soliton is normalised on the two-dimensional lattice and so the field of the effective one-dimensional soliton is normalised to $\frac{1}{N_y}$, where N_y describes

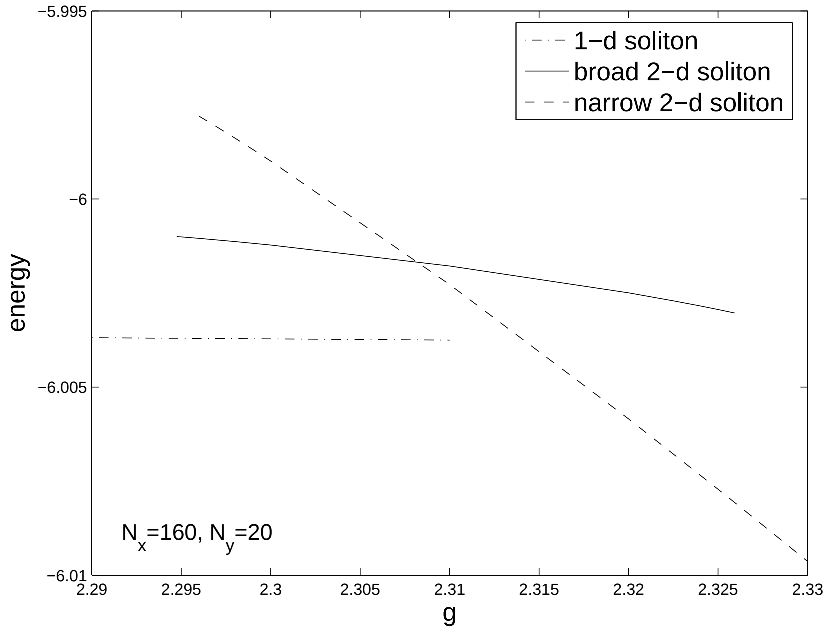

Figure 4. The energy of the two-dimensional narrow, respectively, broad solitons in comparsion with the energy of the one-d soliton. Note that the energy of the configuration with equally distributed $\psi_{i,j}\psi^*_{i,j} = 1/(160 \cdot 20)$ would have energy ≈ -5.8576.

the number of points in the "shorter" direction). A simple scaling argument then explains the observed N_y dependence of the critical value of the electron-phonon coupling constant for the existence of one-dimensional solitons.

Though our investigations were performed only for the 2-dimensional hexagonal lattice, we would expect that similar features appear in the case of other lattice structures, i.e. lattices in physical three dimensional spaces, the quadratic lattices of [1, 3, 2] etc.

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References

[1] Brizhik L, Eremko A, Piette B and Zakrzewski W J, *Physica D* **146** (2000), 275.

[2] Brizhik L, Piette B and Zakrzewski W J, *Ukr. Fiz. Journal* **46** (2001), 503.

[3] Brizhik L, Eremko A, Piette B and Zakrzewski W J, *Physica D* **159** (2001), 71.

[4] Hartmann B and Zakrzewski W J, *Phys. Rev. B* **68** (2003), 184302.

[5] Davydov A S, Solitons in molecular systems, Reidel, Dordrecht, 1985.

[6] Scott A, *Phys. Rep.* **217** (1992), 1; Nonlinear excitations in Biomolecules, Editor: Peyrard M, Springer, Berlin, 1996.