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Electrons on hexagonal lattices and applications to nanotubes

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We consider a Fröhlich-type Hamiltonian on a hexagonal lattice. Aiming to describe nanotubes, we choose this two-dimensional lattice to be periodic and to have a large extension in one (x) direction and a small extension in the other (y) direction. We study the existence of solitons in this model using both analytical and numerical methods. We find exact solutions of our equations and discuss some of their properties.

I. INTRODUCTION

Nanotubes have attracted a large amount of interest ever since they were first discovered in 1991.1 They can be thought of as carbon cylinders with a hexagonal grid and are thus fullerene related structures. Their mechanical, thermal, optical, and electrical properties have been studied in some detail.2 It was found that most properties depend crucially on optical, and electrical properties have been studied in some thought of as carbon cylinders with a hexagonal grid and are external force such as, e.g., bending, stretching, or the lattice thus affects the energy-band gap. This distortion of the diameter, chirality, and length of the tube. A distortion of dimensional, discrete, quadratic lattice. 6–8 In Refs. 6 and 7, ~

firmed these results8 by showing that in the continuum limit electron-phonon coupling constant. An analytical study con-

the existence of localized states was studied numerically and an excitation such as an amide ~5 in 1970s to explain the dispersion-
lattice whose distortion is initially caused by the excitation an electron

~

vibration in biopolymers or

introduced by Davydov4 in 1970s to explain the dispersion-

and chirality could be constructed in our model.

II. THE HAMILTONIAN AND EQUATIONS OF MOTION

A. Hamiltonian

The Hamiltonian H of our model is a sum of four sums which result from the special features of the hexagonal grid. ψi,j denotes the electron field on the ith and the jth lattice side, while ui,j and vi,j are the displacements of the ith and the jth lattice point from equilibrium in the x and y directions, respectively:

\[
H = \sum_{(i-j)/2=0}^{(N_{j}/2)-1} \sum_{(i-j)/4=0}^{(N_{i}/4)-3} \left[ (E + W) \psi_{i,j} \psi_{i,j}^\dagger - j_x \psi_{i,j}^\dagger (\psi_{i+1,j+1} + \psi_{i-1,j+1} + \psi_{i+1,j-1} + \psi_{i-1,j-1}) - j_x \psi_{i,j} (\psi_{i+1,j+1}^\dagger + \psi_{i-1,j+1}^\dagger + \psi_{i+1,j-1}^\dagger + \psi_{i-1,j-1}^\dagger) \right] + \sum_{(i-j)/2=1}^{(N_{j}/2)-2} \sum_{(i-j)/4=0}^{(N_{i}/4)-2} (E + W) \psi_{i,j} \psi_{i,j}^\dagger
\]

\[
+ j_x \psi_{i,j}^\dagger (\psi_{i+1,j+1} + \psi_{i-1,j+1} + \psi_{i+1,j-1} + \psi_{i-1,j-1}) - j_x \psi_{i,j} (\psi_{i+1,j+1}^\dagger + \psi_{i-1,j+1}^\dagger + \psi_{i+1,j-1}^\dagger + \psi_{i-1,j-1}^\dagger) + |\psi_{i,j}|^2
\]

\[
\times \left[ c_x (u_{i-1,j+1} - u_{i-1,j-1} + 2u_{i+1,j}) + c_x (v_{i-1,j+1} - v_{i-1,j-1}) \right]
\]

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j_x is the electron field self-interaction coupling, c_x couples the electron field to the displacement fields u and v, and k_x is the self-coupling of the displacement fields.

**B. Equations of motion**

We can easily derive the equations of motion from our Hamiltonian $H$. As an example, we give the equations for $i = 1 + 4k$. The discrete Schrödinger equation for the $\psi_{i,j}$ field thus becomes

$$i\hbar \frac{\partial \psi_{i,j}}{\partial t} = (E + W) \psi_{i,j} - j_x \psi_{i+1,j+1} + \psi_{i-1,j} + \psi_{i+1,j-1}$$

$$+ \psi_{i,j} \left[ \frac{c_x}{3} (u_{i+1,j+1} + u_{i+1,j-1} - 2u_{i-1,j}) \right]$$

$$+ \psi_{i,j} \left[ \frac{c_x}{\sqrt{3}} (v_{i+1,j+1} - v_{i+1,j-1}) \right],$$

while the equations for the displacement fields $u_{i,j}$ and $v_{i,j}$ are given by

$$\frac{d^2 u_{i,j}}{dt^2} = k_x (3u_{i,j} - u_{i+1,j+1} - u_{i-1,j} - u_{i+1,j-1})$$

$$+ \frac{c_x}{3M} (2|\psi_{i-1,j}|^2 - |\psi_{i+1,j+1}|^2 - |\psi_{i+1,j-1}|^2),$$

and

$$\frac{d^2 v_{i,j}}{dt^2} = k_x (3v_{i,j} - v_{i+1,j+1} - v_{i-1,j} - v_{i+1,j-1})$$

$$- \frac{c_x}{3M} (|\psi_{i+1,j+1}|^2 - |\psi_{i+1,j-1}|^2).$$

We perform the following rescalings:

$$\tau = \frac{j_x t}{\hbar}, \quad U = 3C_x u, \quad V = 3C_x v, \quad E_0 = \frac{E}{j_x}, \quad W_0 = \frac{W}{j_x}$$

and introduce the following rescaled coupling constants:
\[
C_x = \frac{c_x}{j_x}, \quad K_x = \frac{k_x h^2}{j_x^2}, \quad g = \frac{2C_x^2}{E_x}, \quad E_x = \frac{M j_x}{9 h^2}. \tag{7}
\]

The equations then read
\[
\begin{aligned}
d\psi_{i,j}/dt &= (E_0 + W_0) \psi_{i,j} - 2(\psi_{i+1,j+1} + \psi_{i-1,j} + \psi_{i+1,j-1}) \\
&+ \psi_{i,j}(U_{i+1,j+1} + U_{i+1,j-1} - 2U_{i-1,j}) \\
&+ \sqrt{3}(V_{i+1,j+1} - V_{i+1,j-1}),
\end{aligned}
\tag{8}
\]
\[
d^2U_{i,j}/d\tau^2 = K_x(3U_{i,j} - U_{i+1,j+1} - U_{i-1,j} - U_{i+1,j-1}) \\
+ \frac{g}{2}(2|\psi_{i-1,j}|^2 - |\psi_{i+1,j+1}|^2 - |\psi_{i+1,j-1}|^2), \tag{9}
\]
\[
d^2V_{i,j}/d\tau^2 = K_x(3V_{i,j} - V_{i+1,j+1} - V_{i-1,j} - V_{i+1,j-1}) \\
- \frac{\sqrt{3}g}{2}(|\psi_{i+1,j+1}|^2 - |\psi_{i+1,j-1}|^2). \tag{10}
\]

### III. STATIONARY LIMIT

In the stationary limit, we have
\[
\begin{aligned}
\lambda \psi_{i,j} &+ 2(3\psi_{i,j} - \psi_{i+1,j+1} - \psi_{i-1,j} - \psi_{i+1,j-1}) \\
&+ \psi_{i,j}(U_{i+1,j+1} + U_{i+1,j-1} - 2U_{i-1,j}) \\
&+ \sqrt{3}(V_{i+1,j+1} - V_{i+1,j-1}) = 0, \tag{11}
\end{aligned}
\]
where \(\lambda = E_0 + W_0 - 6\) and
\[
\begin{aligned}
3U_{i,j} - U_{i+1,j+1} - U_{i-1,j} - U_{i+1,j-1} &= -\frac{g}{2}(2|\psi_{i-1,j}|^2 - |\psi_{i+1,j+1}|^2 - |\psi_{i+1,j-1}|^2), \tag{12}
\end{aligned}
\]
\[
\begin{aligned}
3V_{i,j} - V_{i+1,j+1} - V_{i-1,j} - V_{i+1,j-1} &= \frac{\sqrt{3}g}{2}(|\psi_{i+1,j+1}|^2 - |\psi_{i+1,j-1}|^2). \tag{13}
\end{aligned}
\]
where \(\tilde{g} = g/K_x\).

### A. Discrete equation

In contrast to the square grid, we find that the discrete equations of the hexagonal grid in the stationary limit do have an exact solution. We can thus replace the system of coupled equations (3)–(5) by just one modified DNLS equation. We again look at the case \(i = 1 + 4k\) for which we have
\[
\Delta(1)U_{i,j} = \tilde{g}(2|\psi_{i-1,j}|^2 - |\psi_{i+1,j+1}|^2 - |\psi_{i+1,j-1}|^2),
\]
where \(\Delta(1)U_{i,j} = U_{i+1,j+1} + U_{i+1,j-1} - 3U_{i,j}\).

Analogously, we have
\[
\Delta(1)V_{i,j} = \frac{\sqrt{3}\tilde{g}}{2}(|\psi_{i+1,j-1}|^2 - |\psi_{i+1,j+1}|^2),
\]
where \(\Delta(1)V_{i,j} = V_{i+1,j+1} + V_{i+1,j-1} - 3V_{i,j}\). Next we note that for the three nearest neighbors we have similar relations, namely,
\[
\Delta(1)U_{i+1,j+1} = \tilde{g}(|\psi_{i,j}|^2 + |\psi_{i,j+2}|^2 - 2|\psi_{i+2,j+1}|^2),
\]
\[
\Delta(1)U_{i+1,j-1} = \tilde{g}(|\psi_{i,j-2}|^2 + |\psi_{i,j}|^2 - 2|\psi_{i+2,j-1}|^2),
\]
\[
\Delta(1)V_{i-1,j-1} = \frac{\sqrt{3}\tilde{g}}{2}(|\psi_{i-2,j-1}|^2 + |\psi_{i-2,j+1}|^2 - 2|\psi_{i,j}|^2)
\]
for the \(U\) field and
\[
\Delta(1)V_{i+1,j+1} = \frac{\sqrt{3}\tilde{g}}{2}(|\psi_{i,j}|^2 - |\psi_{i,j+2}|^2),
\]
\[
\Delta(1)V_{i+1,j-1} = \frac{\sqrt{3}\tilde{g}}{2}(|\psi_{i,j-2}|^2 - |\psi_{i,j}|^2)
\]
for the \(V\) field.

Defining
\[
Z_a = U_{i+1,j+1} + U_{i+1,j-1} - 2U_{i,j} + \sqrt{3}(V_{i+1,j+1} - V_{i+1,j-1})
\]
[i.e., the lattice terms in Eq. (11)] we find that the following discrete equation holds:
\[
\Delta(1)Z_a = \tilde{g}(6|\psi_{i,j}|^2 - |\psi_{i,j+2}|^2 - |\psi_{i+2,j+1}|^2 - |\psi_{i,j-2}|^2 - |\psi_{i+2,j-1}|^2 - |\psi_{i,j+2}|^2). \tag{14}
\]

The right-hand side of Eq. (14) is a seven-point Laplacian \(\Delta(2)|\psi_{i,j}|^2\), thus we find
\[
\Delta(1)Z_a = -\tilde{g}\Delta(2)|\psi_{i,j}|^2. \tag{15}
\]

It is easy to see that one possible solution of this equation is of the form
\[
Z_a = -\tilde{g}(|\psi_{i+1,j+1}|^2 + |\psi_{i+1,j-1}|^2 + |\psi_{i-1,j}|^2 + 3|\psi_{i,j}|^2).
\]

This is quite remarkable since on a square lattice a similar equation has no simple solution. Inserting Eq. (15) into Eq. (11) we have
\[
\lambda \psi_{i,j} + 2(3 \psi_{i,j} - \psi_{i+1,j+1} - \psi_{i-1,j} - \psi_{i+1,j-1}) \\
- \bar{g} \psi_{i,j}[|\psi_{i+1,j+1}|^2 + |\psi_{i+1,j-1}|^2 + |\psi_{i-1,j}|^2 + 3|\psi_{i,j}|^2] \\
= 0
\]

or

\[
\lambda \psi_{i,j} - 2\Delta (1) \psi_{i,j} - \bar{g} \psi_{i,j}(\Delta (1)|\psi_{i,j}|^2 + 6|\psi_{i,j}|^2) = 0.
\]

This equation constitutes our DNLS equation.

B. Continuum limit

Next we look at the continuum limit of Eq. (16). To do this we introduce the following expansions:

\[
\psi_{i \pm 1,j+1} = \psi \pm \delta x \frac{\partial \psi}{\partial x} + \delta y \frac{\partial \psi}{\partial y} + \frac{1}{2} (\delta x_{\pm})^2 \frac{\partial^2 \psi}{\partial x^2} \\
+ \delta y \delta x_{\pm} \frac{\partial^2 \psi}{\partial x \partial y} + \frac{1}{2} (\delta y_{\pm})^2 \frac{\partial^2 \psi}{\partial y^2} + \frac{1}{8} (\delta x_{\pm})^3 \frac{\partial^3 \psi}{\partial x^3} \\
+ \frac{1}{2} (\delta x_{\pm})^2 \delta y \frac{\partial^3 \psi}{\partial x^2 \partial y} + \frac{1}{2} \delta x_{\pm} \delta y (\delta y_{\pm})^2 \frac{\partial^3 \psi}{\partial x \partial y^2} \\
+ \frac{1}{8} (\delta y_{\pm})^3 \frac{\partial^3 \psi}{\partial y^3} \pm \cdots
\]

and

\[
\psi_{i \pm 1,j-1} = \psi \pm \delta x \frac{\partial \psi}{\partial x} - \delta y \frac{\partial \psi}{\partial y} + \frac{1}{2} (\delta x_{\pm})^2 \frac{\partial^2 \psi}{\partial x^2} \\
+ \delta y \delta x_{\pm} \frac{\partial^2 \psi}{\partial x \partial y} + \frac{1}{2} (\delta y_{\pm})^2 \frac{\partial^2 \psi}{\partial y^2} + \frac{1}{8} (\delta x_{\pm})^3 \frac{\partial^3 \psi}{\partial x^3} \\
- \frac{1}{2} (\delta x_{\pm})^2 \delta y \frac{\partial^3 \psi}{\partial x^2 \partial y} + \frac{1}{2} \delta x_{\pm} \delta y (\delta y_{\pm})^2 \frac{\partial^3 \psi}{\partial x \partial y^2} \\
- \frac{1}{8} (\delta y_{\pm})^3 \frac{\partial^3 \psi}{\partial y^3} \pm \cdots
\]

where for \(i = 1 + 4k\) and \(i = 3 + 4k\) we have \(\delta x_+ = 1/2, \delta x_- = 1\), while for \(i = 2 + 4k\) and \(i = 4 + 4k\) we have \(\delta x_+ = 1, \delta x_- = 1/2\). Moreover, \(\delta y = \sqrt{3}/2\). Inserting this into Eq. (16), we obtain

\[
\lambda \psi - \frac{3}{2} \Delta \psi - \bar{g} \psi \left( \frac{3}{4} \Delta |\psi|^2 + 6 |\psi|^2 \right) = 0
\]

or, equivalently,

\[
\bar{\lambda} \psi + \Delta \psi + 4 \bar{g} \psi \left( |\psi|^2 + \frac{1}{8} \Delta |\psi|^2 \right) = 0.
\]

We thus have, in analogy to what was found in Refs. 6–8, the MNLS equation with an extra term, which can stabilize the soliton:

\[
\frac{\partial \psi}{\partial \tau} + \Delta \psi + 4 \bar{g} \psi \left( |\psi|^2 + \frac{1}{8} \Delta |\psi|^2 \right) = 0.
\]
similar to that for Q-balls, we have an extra term involving derivatives as compared to an “ordinary” $\psi^6$-potential in the case of Q-balls.

B. Discrete equations

1. Full system of equations

For our numerical study of the full equations (3)–(5) we have found it convenient to “squeeze” the lattice as indicated in Figs. 2(a) and 2(b). The Hamiltonian and the corresponding equations are given in the Appendix. For our numerical calculations, we have used mainly a periodic grid with $N_1 = 160$ and $N_2 = 20$. We have in addition chosen the boundary conditions such that the fields at $(i = 0, j)$ are identified with those at $(i = i_{\text{max}}, j)$. Thus the type of nanotube we are studying here is a (5,5) armchair tube which is metallic. Nanotubes can also be semiconducting and we make a brief comment about the possibility of constructing semiconducting tubes in our model in the last paragraph of this section.

In this work, the C—C bond length, 0.1415 nm, is normalized to unity. Therefore, the tube diameter is 0.6756 nm. Tubes with different diameter can also be constructed in our model. We discuss this together with different chiralities in the last paragraph of this section.

As starting configuration we have used an exponential-like excitation $\psi_{i,j}$ extended typically over the lattice points $i = 78–83$ and $j = 3–7$ with the lattice at equilibrium everywhere, i.e., $u_{i,j} = 0$ and $v_{i,j} = 0$ for all $i,j$. We are mainly interested in the existence of solitons and their dependence on the value of the coupling constant $c_x$. We have set $j_x = k_x = 1$, $M = 20$, and $E = 0.142 \, 312$. The main goal of this work is to study the dependence on $c_x$. So the exact values of $j_x$ and $k_x$ play a minor role. Hence, we have set them to one. The choice of $M = 20$ is a reflection of the physical fact that the mass of the carbon atom is $\approx 20 \times 10^{-24} \, g$.

To absorb the energy thus allowing the initial configuration to evolve into the stationary solutions of Eqs. (3)–(5), i.e., of Eqs. (11)–(13) we have additionally introduced damping terms $\nu (du_{i,j}/dt)$ and $\nu (dv_{i,j}/dt)$, respectively, into Eqs. (4) and (5). We have typically chosen $\nu = 0.25 – 0.75$. For this choice of the coupling constants, we have performed several numerical calculations using a fourth-order Runge-Kutta method for simulating the time evolution. We have found that solitons exist in this system for $c_x > -20$. For larger values of $c_x$, the soliton forms very quickly, while decreasing $c_x$ the time increases at which a
soliton forms. This is of course due to the weaker coupling between the dynamics of the lattice itself and the excitation. For $c_s = 19$, we have waited until $t \approx 8000$ and have not found a soliton. Moreover, in all cases we have found only little displacement of the lattice from the equilibrium. We have found that at the location of the soliton the lattice becomes squeezed (i.e., the lattice sites move towards the sites at which the soliton is located). This is demonstrated in Fig. 3 for $c_s = 25$, where we show the lattice distortion after $t = 4000$. The point at which the center of the soliton is located does not move, while the sites in its close neighborhood all move towards the center of the soliton.

We have also studied the effects of perturbations of the solitons. We have found that after perturbing the soliton we obtain a new solution with a different height of the soliton maximum. Even after introducing a perturbation which keeps the maximal height fixed, the new solution differs from the starting one. We thus come to the conclusion that the full system of Eqs. (3)–(5) has a large number of solutions for each choice of coupling constants. We believe that a conserved quantity exists in this system which picks out the specific solution. However, so far we have not been able to determine this conserved quantity.

2. Modified, discrete nonlinear Schrödinger equation

In addition to the full system of equations, we have also studied the dynamical analog of Eq. (16). Using a similar starting configuration with $\psi_{i,j}$ being exponential and non-zero over $i = 78–83$ and $j = 3–7$, we have determined the value of $\tilde{g}$ for which a soliton exists. Our results are shown in Fig. 4, where we present the height of the soliton’s maximum $(\psi \psi^*)_{\text{max}}$ as function of $\tilde{g}$. We find that the value of $\tilde{g}$ at which the soliton disappears $g_{cr} \approx 2.295$. The height of the soliton at this critical coupling is $(\psi_{i,j} \psi_{i,j}^*)_{\text{max}} \approx 0.227$. Our numerical study of the continuous MNLS equation gave us $g_{cr} \approx 2.94$, while the analytical study led to $\tilde{g}_{cr} = \pi$. Both values are not a bad approximation for the value found numerically for the discrete equation.

To test the independence of our results from the form of the initial settings, we have used a different starting configuration with two exponential-like excitations being located at $i = 78–83$, $j = 3–7$ and $i = 138–143$ and $j = 13–17$, respectively. We have found that for values $\tilde{g} > 3$, the results agree. For both types of initial configurations, the minimal energy configuration corresponds to one soliton. However, having said this, the time to reach this minimal energy configuration is significantly smaller for the initial configuration with one excitation than for that with two excitations (typically one order of magnitude smaller). We have also tested our results as to the dependence on the size of the grid. For this, we have chosen two excitations on three different grid sizes: (a) a grid with $N_1 = 160$, $N_2 = 20$, and two exponential excitations extended over $i = 78–83$, $j = 3–7$ and $i = 138–143$, $j = 13–17$, respectively, (b) a grid with $N_1 = 320$ and $N_2 = 40$ with the excitations located at the same places as in (a), and (c) a grid with $N_1 = 60$, $N_2 = 10$, and two exponential excitations extended over $i = 18–23$, $j = 2–4$ and $i = 38–43$, $j = 7–9$, respectively. We have found that for $\tilde{g} = 3$, the results of cases (a) and (c) agree. For the case (a) the soliton forms at $t \approx 300$, while for the case (c) it forms at $t = 100$. This is not surprising since in the case (c), the two excitations are located nearer to each other than in the case (a). To test the dependence on the actual lattice size we have compared the cases (a) and (b). We have found that for the larger lattice the longer it takes for the soliton to form. For $\tilde{g} = 3$ a soliton forms after $t \approx 300$ in the case (a), while for (b) it forms at $t > 700$. We have thus found that, in comparison with the case of the full system of equations, the solutions of the DNLS equation are unique for each choice of the coupling constant.

![FIG. 3. The distortion of the lattice close to the location of the soliton is shown. The squares indicate the undistorted lattice, while the circles indicate the distorted lattice after $t = 4000$; $c_s = 25$. The corresponding soliton’s maximum $(\psi \psi^*)_{\text{max}} \approx 0.6145$.](image3)

![FIG. 4. The height of the soliton’s maximum $(\psi_{i,j} \psi_{i,j}^*)_{\text{max}}$ is shown as a function of the parameter $\tilde{g}$.](image4)
3. Comparison of results

Since we have found that in the stationary limit the full system of equations can be replaced by the DNLS equation, the minimal energy solutions we have obtained for both types of equations should be in agreement.

Comparing the two systems, we see that the value $\tilde{c}$ is given in terms of the coupling constants of the full system by

$$\tilde{c} = \frac{2}{9} \frac{c_s^2}{M_j k_s},$$

which, for the choice of coupling constants we have used in our numerical simulations, gives

$$\tilde{c} = \frac{c_s^2}{90}. \quad (27)$$

Thus a critical value of $c_s = 20$ would imply $\tilde{g}_{cr} = 4.4$. First, we remark that the values of the critical electron-phonon coupling we obtained from all our simulations (including those for the continuous MNLS equation) are of the same order of magnitude. However, there is a slight discrepancy between the results for the full system and the DNLS equation. We believe that this is due to the fact that there might exist additional terms $A$ in Eq. (15) for which $\Delta(1)A = 0$ and/or $\Delta(2)A = 0$. These terms would then appear in Eq. (16) and would change the comparison of the solutions. However, it is difficult to determine these additional terms and so this is left as a future work.\textsuperscript{13}

4. Tubes with different diameter, chirality, and lengths

Since most of our results are for a (5,5) armchair tube and since it is well known that the properties of nanotubes depend strongly on the diameter, chirality, and lengths of the tube, we will discuss briefly how different tubes could be constructed in our model. We have not constructed these tubes yet, but we aim to do so in a future publication in which we intend to extend our approach to a more realistic three-dimensional model.\textsuperscript{13}

Labeling the first carbon atom in the $y$ direction by $j = 0$, we have chosen $j_{\text{max}}$, such that it is divisible by 4. Thus, the length of the tube in the $y$ direction is $l_y = \frac{1}{4} j_{\text{max}}$. Since we identify the fields labeled by $(i = 0, j)$ with those at $(i = i_{\text{max}}, j)$, the diameter of the tube is given by $d = l_y / \pi$. Thus increasing/decreasing $j_{\text{max}}$ by $4n$, $n = 1, 2, 3, \ldots$, we can construct armchair nanotubes with diameters $d = (3/4 \pi) (j_{\text{max}} \pm 4n)$. Similarly, we can construct longer tubes by increasing the number of atoms in the $x$ direction.

As far as chirality is concerned, there are two things to modify in our model in order to be able to construct tubes with different chirality. One is to change the number of points in the $y$ direction so that $j_{\text{max}}$ is nondivisible by 4. The other is to adjust the periodic boundary conditions in the $y$ direction appropriately. If we, e.g., choose $j_{\text{max}} = 18$, we have to identify the fields at $(i = 0, j)$ with those at $(i = i_{\text{max}}, j + 1)$. This then would give us a (5,4) nanotube which would be semiconducting.

In this work, we have concentrated our attention on the existence of localized structures. These structures extend over large parts of our grids, but are negligible at boundaries. Hence, we expect these to hold for systems with different boundary conditions, i.e., different chiralities.

V. CONCLUSIONS

Motivated by a large amount of research done in the area of nanotubes, we have studied solitons on a two-dimensional hexagonal lattice. We have chosen our lattice to be periodic in both the $x$ and $y$ directions and to be of large extension in one $(x)$ direction and of small extension in the other $(y)$ direction. In the stationary limit, we have found that the full system of equations in which the electron excitation is coupled to the displacement fields of the lattice can be replaced by a modified discrete nonlinear Schrödinger (DNLS) equation. This discovery of an exact solution of the full system of equations is remarkable since for the similar quadratic lattice such a simple solution does not exist.

In our numerical studies we have mainly concentrated our attention on determining the value of the critical phonon-electron coupling constant. For the DNLS we have found that unique solutions exist and that the value of the critical coupling is in good agreement with both the analytical and numerical values found for the continuous analog of the DNLS. For the full system of equations, we believe that a large number of solutions exist for each choice of the coupling constants and that a conserved quantity exists in the system. The critical value of the electron-phonon coupling is of the same order of magnitude as in the case of the DNLS; however, we believe that this small discrepancy results from the fact that possible “boundary” terms appear when replacing the full system by the DNLS. These boundary terms are that which are annihilated by either the four-point Laplacian $\Delta(1)$ and/or by the seven-point Laplacian $\Delta(2)$. To find these terms is nontrivial and since this seems an interesting topic by itself, we leave this as a future work.\textsuperscript{13}

Finally let us mention that a possible extension of the results given here would involve the study of the corresponding three-dimensional equations and/or of the influence of external forces.

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APPENDIX: HAMILTONIAN AND EQUATIONS OF MOTION FOR THE NUMERICAL STUDIES

To simplify the numerical construction of the solutions we have squeezed the lattice as indicated in Figs. 2(a) and 2(b). This reduces the memory requirements and so speeds up the calculations. The Hamiltonian $H^n$ for the numerical construction thus takes the form
\[ H^p = \sum_{j=1}^{N_z} \sum_{(i-1)4^3=0}^{(N_z/4)-3} \left( (E + W) \psi_{i,j} \psi_{i,j}^* - j_x \psi_{i,j} \left( \psi_{i+1,j}^* + \psi_{i-1,j} + \psi_{i+1,j-1} \right) \right) \]
\[ - j_x \psi_{i,j} \left( \psi_{i+1,j}^* + \psi_{i-1,j} + \psi_{i+1,j-1} \right) + \psi_{i,j} \psi_{i,j}^* \left( \frac{c_s}{3} (u_{i+1,j} + u_{i+1,j-1} + 2u_{i-1,j}) - \frac{c_s}{\sqrt{3}} (v_{i+1,j-1} - v_{i+1,j}) \right) \]
\[ + \sum_{j=1}^{N_z} \sum_{(i-2)4^3=0}^{(N_z/4)-2} \left( (E + W) \psi_{i,j} \psi_{i,j}^* - j_x \psi_{i,j} \left( \psi_{i+1,j}^* + \psi_{i-1,j} + \psi_{i-1,j+1} \right) \right) \]
\[ - j_x \psi_{i,j} \left( \psi_{i+1,j}^* + \psi_{i-1,j} + \psi_{i-1,j+1} \right) + \psi_{i,j} \psi_{i,j}^* \left( \frac{c_s}{3} (-u_{i-1,j} - u_{i-1,j+1} + 2u_{i+1,j}) + \frac{c_s}{\sqrt{3}} (v_{i-1,j+1} - v_{i-1,j}) \right) \]
\[ + \sum_{j=1}^{N_z} \sum_{(i-3)4^3=0}^{(N_z/4)-1} \left( (E + W) \psi_{i,j} \psi_{i,j}^* - j_x \psi_{i,j} \left( \psi_{i+1,j}^* + \psi_{i-1,j} + \psi_{i-1,j+1} \right) \right) \]
\[ - j_x \psi_{i,j} \left( \psi_{i+1,j}^* + \psi_{i-1,j} + \psi_{i-1,j+1} \right) + \psi_{i,j} \psi_{i,j}^* \left( \frac{c_s}{3} (u_{i+1,j} + u_{i+1,j-1} - 2u_{i-1,j}) + \frac{c_s}{\sqrt{3}} (v_{i+1,j+1} - v_{i+1,j}) \right) \]
\[ + \sum_{j=1}^{N_z} \sum_{i4^3=1}^{N_z} \left( (E + W) \psi_{i,j} \psi_{i,j}^* - j_x \psi_{i,j} \left( \psi_{i+1,j}^* + \psi_{i-1,j} + \psi_{i-1,j-1} \right) \right) \]
\[ - j_x \psi_{i,j} \left( \psi_{i+1,j}^* + \psi_{i-1,j} + \psi_{i-1,j-1} \right) + \psi_{i,j} \psi_{i,j}^* \left( \frac{c_s}{3} (u_{i-1,j} + u_{i-1,j-1} - 2u_{i+1,j}) + \frac{c_s}{\sqrt{3}} (v_{i-1,j+1} - v_{i-1,j}) \right) \]
\[ \text{(A1)} \]

with the phonon energy \( W^p \),

\[ W^p = \frac{1}{2} M \sum_{j=1}^{N_z} \sum_{i4^3=1}^{N_z} \left[ \left( \frac{du_{i,j}}{dt} \right)^2 + \left( \frac{dv_{i,j}}{dt} \right)^2 + k_s \left( u_{i,j} - u_{i-1,j} \right)^2 + (v_{i,j} - v_{i-1,j})^2 \right] + \frac{1}{2} M \sum_{j=1}^{N_z} \sum_{(i-1)4^3=0}^{(N_z/4)-2} \left( k_s \left( u_{i,j} - u_{i-1,j} \right)^2 + (v_{i,j} - v_{i-1,j+1})^2 \right) \]

\[ + \frac{1}{2} M \sum_{j=1}^{N_z} \sum_{(i-3)4^3=0}^{(N_z/4)-1} \left( k_s \left( u_{i,j} - u_{i+1,j+1} \right)^2 + (v_{i,j} - v_{i+1,j+1})^2 \right). \]

\[ \text{(A2)} \]

The equations of motion are then given by

For \( i = 1 + 4k, k = 1, 2, \ldots \),

\[ i \hbar \frac{\partial \psi_{i,j}}{\partial t} = (E + W) \psi_{i,j} - 2j_x (\psi_{i+1,j} + \psi_{i-1,j} + \psi_{i+1,j-1}) + \psi_{i,j} \left[ \frac{c_s}{3} (u_{i+1,j} + u_{i+1,j-1} - 2u_{i-1,j}) + \frac{c_s}{\sqrt{3}} (v_{i+1,j+1} - v_{i+1,j}) \right], \]

\[ \text{(A3)} \]

For \( i = 2 + 4k, k = 1, 2, \ldots \),

\[ i \hbar \frac{\partial \psi_{i,j}}{\partial t} = (E + W) \psi_{i,j} - 2j_x (\psi_{i+1,j} + \psi_{i-1,j} + \psi_{i-1,j+1}) + \psi_{i,j} \left[ \frac{c_s}{3} (-u_{i-1,j} - u_{i-1,j+1} + 2u_{i+1,j}) + \frac{c_s}{\sqrt{3}} (v_{i-1,j+1} - v_{i-1,j}) \right]. \]

\[ \text{(A6)} \]
\[ \frac{d^2 u_{i,j}}{dt^2} = -k_x (3u_{i,j} - u_{i+1,j} - u_{i-1,j} - u_{i,j+1}) \]

\[ + \frac{c_x}{3M} (2\psi_{i+1,j}\psi_{i+1,j} - \psi_{i,j}\psi_{i-1,j}) \]

\[ - \psi_{i-1,j-1}\psi_{i-1,j+1} \]  \hspace{1cm} (A7)

\[ \frac{d^2 v_{i,j}}{dt^2} = -k_x (3v_{i,j} - v_{i+1,j} - v_{i-1,j} - v_{i,j+1}) \]

\[ + \frac{c_x}{\sqrt{3}M} (\psi_{i-1,j+1}\psi_{i-1,j+1} - \psi_{i-1,j-1}\psi_{i-1,j-1}) \]  \hspace{1cm} (A8)

For \( i = 3 + 4k \), \( k = 1, 2, \ldots \),

\[ \hbar \frac{\partial \psi_{i,j}}{\partial t} = (E + W) \psi_{i,j} - 2J_x (\psi_{i+1,j} + \psi_{i-1,j} + \psi_{i+1,j+1}) \]

\[ + \psi_{i,j} \left[ \frac{c}{3} (u_{i+1,j} + u_{i+1,j+1} - 2u_{i,j}) \right] \]

\[ + \frac{c_x}{\sqrt{3}} (v_{i+1,j+1} - v_{i,j+1}) \]  \hspace{1cm} (A9)

\[ \frac{d^2 u_{i,j}}{dt^2} = -k_x (3u_{i,j} - u_{i+1,j} - u_{i-1,j} - u_{i,j+1}) \]

\[ - \frac{c_x}{3M} (2\psi_{i-1,j}\psi_{i-1,j} - \psi_{i+1,j}\psi_{i+1,j} - \psi_{i+1,j+1}\psi_{i+1,j+1}) \]  \hspace{1cm} (A10)

\[ \frac{d^2 v_{i,j}}{dt^2} = -k_x (3v_{i,j} - v_{i+1,j} - v_{i-1,j} - v_{i,j+1}) \]

\[ - \frac{c_x}{\sqrt{3}M} (\psi_{i-1,j}\psi_{i-1,j} - \psi_{i-1,j-1}\psi_{i-1,j-1}) \]  \hspace{1cm} (A11)

For \( i = 4 + 4k \), \( k = 1, 2, \ldots \),

\[ \hbar \frac{\partial \psi_{i,j}}{\partial t} = (E + W) \psi_{i,j} - 2J_x (\psi_{i+1,j} + \psi_{i-1,j} + \psi_{i+1,j+1}) \]

\[ - \psi_{i,j} \left[ \frac{c}{3} (u_{i-1,j} + u_{i-1,j-1} - 2u_{i,j}) \right] \]

\[ - \frac{c_x}{\sqrt{3}} (v_{i-1,j-1} - v_{i,j-1}) \]  \hspace{1cm} (A12)

\[ \frac{d^2 u_{i,j}}{dt^2} = -k_x (3u_{i,j} - u_{i+1,j} - u_{i-1,j} - u_{i,j+1}) \]

\[ + \frac{c_x}{3M} (2\psi_{i+1,j}\psi_{i+1,j} - \psi_{i-1,j}\psi_{i-1,j} - \psi_{i+1,j+1}\psi_{i+1,j+1}) \]  \hspace{1cm} (A13)

\[ \frac{d^2 v_{i,j}}{dt^2} = -k_x (3v_{i,j} - v_{i+1,j} - v_{i-1,j} - v_{i,j+1}) \]

\[ + \frac{c_x}{\sqrt{3}M} (\psi_{i+1,j}\psi_{i+1,j} - \psi_{i+1,j-1}\psi_{i+1,j-1}) \]  \hspace{1cm} (A14)