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Solitons on two-dimensional anharmonic square lattices

Tatyana Yu Astakhova and George A Vinogradov

N M Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, ul. Kosygina 4, Moscow 119991 GSP-1, Russia

E-mail: astakhova@deom.chph.ras.ru and gvin@deom.chph.ras.ru

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Abstract
In this paper we consider a square lattice with three types of interactions—nonlinear pair interaction between nearest neighbours, harmonic diagonal interaction and three-particle interaction. The continuum approximation combined with the reductive perturbation method allows us to derive the Kadomtsev–Petviashvili (KP) equation with the lump-soliton solution. Alternatively, the soliton solution is obtained by the pseudo-spectral method. Special attention is paid to determine the range of parameters where the obtained solution is stable. The existence and stability of soliton solutions is checked and verified in molecular dynamics simulations.

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1. Introduction

Solitons are stable localized excitations travelling without dissipation on a lattice. The first hint of the existence of solitons was made in the classical paper of Fermi, Pasta and Ulam (FPU) [1], where the authors did not find an expected energy equalization between different vibration modes in numerical simulation of one-dimensional nonlinear lattices.

The results of FPU experiments were analysed and explained by Zabusky and Kruskal [2] who considered the FPU problem in the continuum approximation and derived the corresponding Korteweg–de Vries (KdV) equation with the soliton solution.

The KdV equation is a third-order nonlinear partial differential equation (NPDE) having the form

$$\varphi_t + 6\varphi\varphi_x + \beta\varphi_{xxx} = 0 \tag{1}$$

with the one-soliton solution

$$\varphi = 2A^2\,\mathrm{sech}^2[A(x - v_{\mathrm{sol}}t)], \tag{2}$$

where A is a parameter. Equation (2) describes a localized solitary excitation with a half-width $w = 1/A$ and amplitude $2A^2$ travelling with velocity $v_{\rm sol} = 4A^2$. For the FPU chain (1) is derived assuming small displacements from the equilibrium positions of particles in the parent lattice and in the long wavelength limit. Thus, the continuum solution (2) is an approximation for discrete systems, and could be unstable in a certain range of parameter A values. Clearly the soliton solution (2) for the lattice is more stable at smaller values of A and wider half-width w.

Further, it was found that there are other one-dimensional (1D) NPDEs possessing a soliton solution [3], i.e. a localized excitation of a constant shape and travelling with a constant velocity, and the KdV equation is a particular case of the family of exactly solvable equations. These equations were successfully utilized in the description of a variety of different physical systems and processes [4, 7].

The next step was the consideration of two-dimensional (2D) integrable NPDEs, i.e. equations with two spatial variables. Of particular interest is the Kadomtsev–Petviashvili (KP) equation, which is also called the 2D KdV equation. The KP equation has the form

$$(\varphi_t + 6\varphi\varphi_x + \varphi_{xxx})_x = \alpha^2\varphi_{yy}, \tag{3}$$

where x, y are spatial variables. The KP equation is also exactly solvable, but the characteristic features of solution essentially depend on the choice of the value of parameter α^2. If $\alpha^2 = 1$ then (3) is known as the KPI equation and admits the family of solutions, which are localized in all directions and are called lump solitons. The exact N-lump-solitons solution of the KPI equation can be constructed as follows [8]:

$$\varphi(x, y, t) = 2\frac{\partial^2}{\partial x^2}\ln\det A, \tag{4}$$

where A is a $2N \times 2N$ matrix with elements

$$A_{kl} = \left(x + \mathrm{i}p_k y - p_k^2 t + \theta_k\right)\delta_{kl} + \frac{1-\delta_{kl}}{p_k - p_l}2\sqrt{3}, \tag{5}$$

and p_k and θ_l are complex constants, which determine the velocity and the phase of the corresponding soliton; $p_{k+N} = \bar{p}_k$, $\theta_{k+N} = \bar{\theta}_k$. The velocity of the ith soliton is determined by

$$\boldsymbol{v}_{\rm sol} = \{(v_{\rm sol})_x, (v_{\rm sol})_y)\} = \{|p_i|^2, 2\,\mathrm{Im}(p_i)\}. \tag{6}$$

The relation between solutions of KdV (1) and KP (3) equations is discussed in [10].

The numerical analysis of one- and N-soliton solutions (4) was presented in a number of published works [11, 12]. In contrast to KdV equation describing many different physical systems and processes, the area of application of 2D KP equation is not so wide. The KP equation was utilized in description of ion-acoustic modes in hot-electron cold-ion plasmas [13], for description of extreme waves in shallow water [14], for modelling thermodynamic quantities in Coulomb gases [15] and in some other cases. There are a number of published works where the KP equation is obtained through continuum approximation of some 2D lattices [12, 16, 17].

The primary goal of this paper is to analyse a 2D square nonlinear lattice to obtain the soliton solution in the continuum approximation. Soliton solutions are derived in two ways: by reductive perturbation and pseudo-spectral methods. Special attention is paid to determine the range of parameters' values where the corresponding solution is stable.

The paper is organized as follows. In section 2, we describe the model lattice with the minimal set of linear and nonlinear interactions allowing to obtain the soliton solution. In the next section, the KP equation for the lattice is derived in the continuum approximation utilizing the reductive perturbation method [18–21]. We get an analytical expression for the

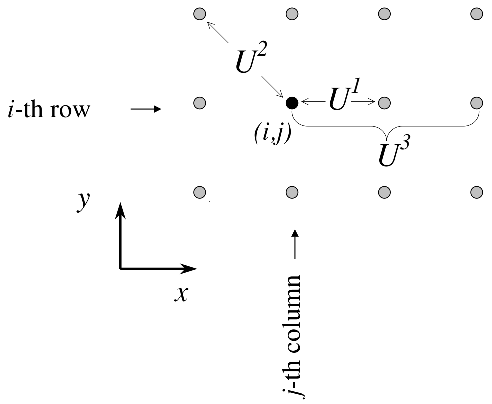

Figure 1. Two-dimensional square lattice.

soliton profile and analyse the range of parameters' values, where the soliton solution is stable. In section 3, we obtain the soliton solution by alternative numerical method—the so-called pseudo-spectral method that was successfully utilized for the description of some 1D and quasi-1D nonlinear structures [22–24]. We compare the obtained solution with results of section 2.2. In section 4, we present the results of numerical simulations of soliton evolution on 2D lattice. The concluding remarks are given in section 5.

2. Two-dimensional lattice and its continuum approximation

2.1. The model

In this paper, we consider $(L \times L)$ square anharmonic lattice, where L is number of rows and columns in the lattice. The coordinate system is shown in figure 1, r_0 is the equilibrium distance between particles along both directions. The position of any particle is determined by a pair of integers (i, j), where i and j numerate particles along rows and columns, respectively.

Let $\boldsymbol{u}_{ij}$ be a deviation of the particle (i, j) from its equilibrium position. Then, its radius-vector is $\boldsymbol{r}_{ij} = \boldsymbol{r}^0_{ij} + \boldsymbol{u}_{ij}$, where $\boldsymbol{r}^0_{ij}$ defines the equilibrium position of the particle and $\boldsymbol{r}^0_{ij} = (ir_0, jr_0)$.

We define the potential energy of the lattice as

$$E = \sum_{ij}[U_1(\boldsymbol{r}_{i,j+1} - \boldsymbol{r}_{i,j}) + U_1(\boldsymbol{r}_{i+1,j} - \boldsymbol{r}_{i,j}) + U_2(\boldsymbol{r}_{i+1,j+1} - \boldsymbol{r}_{i,j}) + U_2(\boldsymbol{r}_{i+1,j-1} - \boldsymbol{r}_{i,j})$$
$$+ U_3(\boldsymbol{r}_{i,j-1} - 2\boldsymbol{r}_{i,j} + \boldsymbol{r}_{i,j+1}) + U_3(\boldsymbol{r}_{i-1,j} - 2\boldsymbol{r}_{i,j} + \boldsymbol{r}_{i+1,j})], \tag{7}$$

where the sum is over all lattice vertices (i, j), and U_1, U_2, U_3 describe nearest neighbour anharmonic, diagonal harmonic and three-body interactions, respectively. U_1, U_2, U_3 have the form

$$U_1(\boldsymbol{r}) = \frac{c_1}{2}(|\boldsymbol{r}| - r_0)^2 - \frac{c_2}{3}(|\boldsymbol{r}| - r_0)^3 \tag{8}$$

$$U_2(\boldsymbol{r}) = \frac{c_3}{2}(|\boldsymbol{r}| - \sqrt{2}r_0)^2 \tag{9}$$

$$U_3(\boldsymbol{r}) = \frac{c_4}{2}|\boldsymbol{r}|^2. \tag{10}$$

2.2. Continuum approximation of 2D lattice and the KP equation

Now we construct the continuum approximation of the 2D lattice described in the previous subsection with the interaction energy given by (7). An analysis shows that solitons, if exist, can travel only along symmetry axes of the lattice. As this takes place, without the loss of generality we consider the particular case when vectors of displacement and their velocities are collinear and aligned along the x-axis: $\boldsymbol{u}_{i,j} = (u_{i,j}, 0)$.

Hereafter we put $r_0 = 1$, making displacements $\boldsymbol{u}_{ij}$ dimensionless, and masses (m) of particles also equal to 1. Assuming small deviations we expand the displacements $\{u_{ij}\}$ into the Taylor series upto the fourth order and get

$$\begin{aligned} u_{km} &= u + u_x k + u_y m + \tfrac{1}{2}(u_{xx}k^2 + u_{xy}km + u_{yy}m^2) \\ &\quad + \tfrac{1}{6}(u_{xxx}k^3 + u_{xxy}k^2m + u_{xyy}km^2 + u_{yyy}m^3) \\ &\quad + \tfrac{1}{24}(u_{xxxx}k^4 + u_{xxxy}k^3m + u_{xxyy}k^2m^2 + u_{xyyy}km^3 + u_{yyyy}m^4), \end{aligned} \tag{11}$$

where $u \equiv u_{ij}, u_{km} \equiv u_{i+kj+m}$ and $k, m = 1, 2$. Then we substitute expansion (11) into the Newtonian equations of motion with potential energy (7) and get

$$\begin{aligned} \ddot{u} &= \left(u_{xx} + \tfrac{1}{12}u_{xxxx}\right) - 2c_2u_xu_{xx} + c_3\left[u_{xx} + u_{yy} + \tfrac{1}{12}(u_{xxxx} + u_{xxyy} + u_{yyyy})\right] \\ &\quad + \tfrac{3}{2}c_3(u_xu_{xx} + u_xu_{yy} + u_yu_{xy}) - c_4(u_{xxxx} + u_{yyyy}). \end{aligned} \tag{12}$$

Next, we follow the generally accepted procedure of the reductive perturbation method (RPM) [18–21] and introduce new variables

$$w = u_x, \qquad v = \dot{u} \tag{13}$$

and expand new variables into series in terms of small value ε

$$w = \varepsilon w_0 + \varepsilon^2 w_1, \ldots, \qquad v = \varepsilon v_0 + \varepsilon^2 v_1, \ldots. \tag{14}$$

Simultaneously, we transform the space and time variables as

$$\xi \equiv \varepsilon^{1/2}(x - ct), \qquad \eta \equiv \varepsilon y, \qquad \tau \equiv \varepsilon^{3/2}t. \tag{15}$$

Equations (14) and (15) mean the following relations of smallness:

$$(w_0)_{\eta\eta} \sim (w_0)_{\xi\xi\xi\xi}, \text{ etc.} \tag{16}$$

If (13)–(15) are substituted into (12) and terms of order ε^2 are set to be zero, one get

$$v_0(\xi, \eta; \tau) = -cw_0(\xi, \eta; \tau) + f(\tau), \tag{17}$$

where

$$c^2 = c_1 + c_3 \tag{18}$$

and $f(\tau)$ is an arbitrary function of τ. We put $f(\tau) = 0$, since we seek a solution so that w tends to zero as $|\xi| \to \infty$ and $|\eta| \to \infty$.

Transformations (15) mean that the new coordinate system $\{\xi, \eta\}$ moves with constant velocity $\boldsymbol{v}_{\xi\eta} = \{c, 0\}$ with respect to the coordinate system $\{x, y\}$, where c is the sound velocity determined by (18).

Equating terms of the order of ε^3 and taking into account (17) and (18), one gets the following equation for w_0:

$$-\left[k_1(w_0)_\tau + k_2w_0(w_0)_\xi + k_3(w_0)_{\xi\xi\xi}\right]_\xi = k_4(w_0)_{\eta\eta}, \tag{19}$$

where $k_1, \ldots, k_4$ are expressed through coefficients of the potential (7):

$$k_1 = 2(c_1 + c_3)^{1/2}, \qquad k_2 = \tfrac{3}{2}c_3 - 2c_2, \qquad k_3 = \tfrac{1}{12}(c_1 + c_3) - c_4, \qquad k_4 = c_3. \tag{20}$$

One can see that (19) has the form of the KP equation, and to get the exact form of the KPI equation (3) with $\alpha^2 = 1$, which has the localized lump soliton solution (4), one should re-scale the parameters:

$$\xi = q_1 \nu, \qquad w_0 = q_2 \varphi, \qquad \tau = q_3 T, \qquad \eta = \mu, \tag{21}$$

where

$$q_1 = \pm \left(-\frac{k_3}{k_4} \right)^{1/4}, \qquad q_2 = -\frac{k_4}{k_2} q_1^2, \qquad q_3 = -\frac{k_1}{k_4 q_1}. \tag{22}$$

Substituting (21) and (22) in (19) one gets the KPI equation (3) for function φ in variables ν, μ, T with N-lump-soliton solution given by (4) and (5). The soliton velocity is determined by (6) and is measured relative to the coordinate system $\{\nu, \mu\}$ moving with the sound velocity c.

2.3. Parameters range of soliton stability

We should be able to make few comments on the values of parameters. All $\{c_i\}, i = 1, \dots, 4$, are expected to be positive by physical reasons. Diagonal interaction should be much smaller compared to harmonic term of nearest neighbour (NN) interactions, i.e. $c_3 \ll c_1$.

Simple analysis of (20) and (22) shows that k_3 must be negative, which means that

$$c_4 > c_1/12. \tag{23}$$

Since c_4 describes the next-nearest neighbour interaction (NNN), it should not be too large. Thus, it is reasonable to choose c_4 in the range $c_4 \approx (0.1 - 0.5)c_1$.

Additional estimations could be done at the analysis of (19). Coefficients k_1, k_4 are positive as c_1 and c_3 are also positive; k_3 is negative to ensure a real value of coefficient q_1, and coefficient k_2 can be either positive or negative. The negative sign of k_2 means that the anharmonic contribution of the NN interaction is larger than the harmonic diagonal interaction, otherwise k_2 is positive. The sign of q_1 is undetermined, which means that the soliton can move either in positive or negative directions of the x-axis.

The sign of q_3 depends on the sign of q_1. Negative sign of q_3 shows that the time variable changes its sign at transformation (21). It means that the coordinate system $\{\nu, \mu\}$ moves along the x-axis of the coordinate system $\{x, y\}$ in the opposite direction as compared to the coordinate system $\{\xi, \eta\}$. The sign of q_2 depends on the sign of the coefficient k_2. Namely, $q_2 > 0$, if $k_2 < 0$, otherwise $q_2 < 0$. Different signs of q_2 depending on the sign of k_2 mean that functions $\varphi(\nu, \mu)$ and $u_x \approx w_0 = q_2\varphi$ have opposite signs and describe the expansion and compression excitations, respectively.

The second and the third terms on the left-hand side of (19) are responsible for the nonlinearity and dispersion, correspondingly. The anharmonism is determined by coefficients c_2 and c_3 (see expression for k_2 in (20)). It means that the diagonal harmonic interaction gives contribution to the effective longitudinal anharmonism (the so-called geometric anharmonicity). This is the reason why one can derive the KPI equation even for $c_2 = 0$, i.e. for purely harmonic NN interaction. But in this case c_3 should be rather large to ensure sufficient anharmonism. On the other hand the diagonal harmonic interaction couples the x and y degrees of freedom, and c_3 should be small to fulfill the condition (16).

Thus, the assumption $c_2 = 0$ results in some contradiction: c_3 should be rather large to ensure sufficient anharmonism, and, on the other hand, it must be small to obey the condition (16).

The analogous situation with geometrical anharmonicity was found in [25], where the 2D lattice of particles interacting via harmonic springs between the nearest and the next-nearest diagonal harmonic interactions was considered.

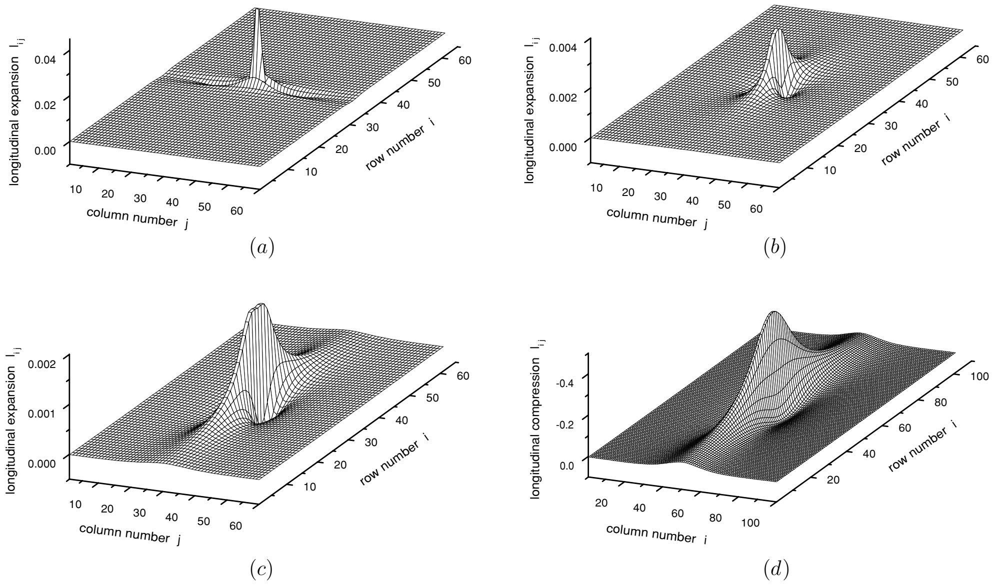

Figure 2. Examples of one-soliton solutions of equation (19) with four sets of potential $\{c_1, c_2, c_3, c_4\}$ and soliton p_1 (see (4) and (5)) parameters: $c_1 = 1.0, c_2 = 10.0, c_3 = 0.01, c_4 = 0.5, p_1 = 0.8$ (*a*); $c_1 = 1.0, c_2 = 10.0, c_3 = 0.02, c_4 = 0.1, p_1 = 0.8$ (*b*); $c_1 = 1.0, c_2 = 10.0, c_3 = 0.05, c_4 = 0.1, p_1 = 0.8$ (*c*); $c_1 = 1.0, c_2 = 0.0, c_3 = 0.5, c_4 = 0.5, p_1 = 0.3$ (*d*). In all cases, the soliton is centred in the geometrical centre of the lattice and solitons move along the rows.

The discussion above on the parameters' choice has a qualitative character and it gives the approximate range of parameters for further numerical analysis.

Figures 2(*a*)–(*d*) show examples of one-soliton analytical solutions of (19) with four sets of parameters $\{c_1, \ldots, c_4\}$ (back transformation to $\{x, y\}$ variables was made). These 3D plots present the distribution of the longitudinal relative inter-particle displacements distance, i.e. $l_{i,j} = u_{i,j+1} - u_{i,j}$.

NN interaction U_1 in (7) is the same in the first three cases (figures 2(*a*)–(*c*)) and $c_2 \neq 0$. Two other parameters c_3 and c_4 vary.

One can see that for the same soliton parameter $p_1 = 0.8$, the soliton profiles and amplitudes are very distinct. The increasing of parameter c_4 results in more narrow and higher soliton. Parameter c_3 is responsible for the soliton width in the y-direction; i.e. the larger is c_3, the wider and lower is the soliton in the y-direction.

Thus, generally speaking, to ensure the soliton stability it is necessary to decrease the value of parameter c_3 and to increase parameter c_4 at constant values of c_1 and c_2.

The case with harmonic potential U_1 ($c_2 = 0$) is presented in figure 2(*d*). In this case, the relative inter-particle displacements change sign and soliton transforms to the expansion soliton with 'negative' amplitude instead of compression soliton for $c_2 \neq 0$.

3. Numerical derivation of soliton solution

Equation (19) was derived in section 2.2 under some assumptions. Firstly, (19) describes the parent 2D lattice at small particles displacements from their equilibrium positions, and in the longwave limit. Additional assumptions were made in deriving the final KP equation by the RPM method. The stability of the KP solution (4) is still questionable and should be additionally checked. There are two ways to be convinced of the soliton stability. The first one is the molecular dynamical (MD) simulations of the soliton evolution on the parent discreet 2D lattice. The second is the so-called pseudo-spectral method (PSM) [22], where the profile of localized soliton-like excitation on a discreet lattice is found numerically. In the PSM, the analytical soliton profile can be chosen as the initial approximation. The PSM was successfully used previously for finding solitary wave solutions in 1D systems [22–24], and we extend this method to 2D systems.

An excitation of a permanent profile travelling with a constant velocity $v_{\rm sol}$ is found in the PSM either by numerical minimization of the corresponding Lagrangian or by the numerical solving of Newtonian equations of motion.

The goal is to find a vector of particles displacements from their equilibrium positions $\boldsymbol{u}(\{x_{ij}, y_{ij}\}, t)$, where $\{x_{ij}, y_{ij}\}$ define the equilibrium position of the particle (i, j), and the displacements satisfy Newtonian equations of motion. Two conditions have to be fulfilled. The desired solution should be localized in both directions (*condition I*) with asymptotics $u(\{x_{ij}, y_{ij}\}, t) \to 0$ for i, j far enough from the soliton centre. The second (*condition II*) means that the desired solution should have a constant profile travelling along the x-direction of the lattice with the velocity $v_{\rm sol}$:

$$\boldsymbol{u}(\{x_{ij}, y_{ij}\}; t) = \boldsymbol{u}(\{\xi_{ij}, \eta_{ij}\}), \qquad \xi_{ij} = x_{ij} - v_{\rm sol} t, \qquad \eta_{ij} = y_{ij}. \tag{24}$$

Condition II (24) allows us to represent the second-order time derivative in the discrete form [23]

$$\ddot{u}_{ij} = v_{\rm sol}^2 \frac{\partial^2 u_{ij}}{\partial \xi_{ij}^2} \approx v_{\rm sol}^2 \frac{-(u_{ij+2} + u_{ij-2}) + 16(u_{ij+1} + u_{ij-1}) - 30u_{ij}}{12}. \tag{25}$$

Taking into account (25), the equations of motion for the 2D lattice with the interaction potential (7), we get

$$v_{\rm sol}^2 \frac{-(u_{ij+2} + u_{ij-2}) + 16(u_{ij+1} + u_{ij-1}) - 30u_{ij}}{12} = -\frac{\partial E_{ij}}{\partial u_{ij}}, \tag{26}$$

where E_{ij} is defined by (7) for $\boldsymbol{r}_{ij} = (u_{ij}, 0)$ $(i, j = 1, \dots, L)$.

It is convenient to search the excitation profile as an expansion into a finite Fourier series:

$$u_{ij} = \sum_{k_1,k_2=1}^{L'} c_{k_1k_2} \cos \frac{2\pi(k_1 - 1)(i - i_{\rm sol} - 1)}{L' - 1} \sin \frac{2\pi(k_2 - 1)(j - j_{\rm sol} - 1)}{L' - 1}, \tag{27}$$

where $L' = L/2$ or $(L+1)/2$ for L even and odd, respectively; $i_{\rm sol}$ and $j_{\rm sol}$ are the coordinates of the soliton centre on the lattice. Substitution of expansion (27) into (26) gives the system of $(L')^2$ nonlinear equations for coefficients $c_{k_1k_2}$.

This system is solved by iteration till the self-consistency in values of expansion coefficients is achieved, taking the analytical soliton solution derived in section 2.2 as an initial approximation.

The soliton profiles calculated by numerical solving of (26) are shown in figure 3. Sets of parameters $\{c_1, \dots, c_4\}$ and the soliton parameter p_1 are chosen in the same manner as in figure 2. The soliton velocity $v_{\rm sol}$ in (26) is calculated using (6) and (21) as

$$v_{\rm sol} = c + \frac{q_1}{q_3}|p_1|^2, \tag{28}$$

where the longitudinal sound velocity c is determined by (18), and coefficients q_1 and q_3 are defined by (22).

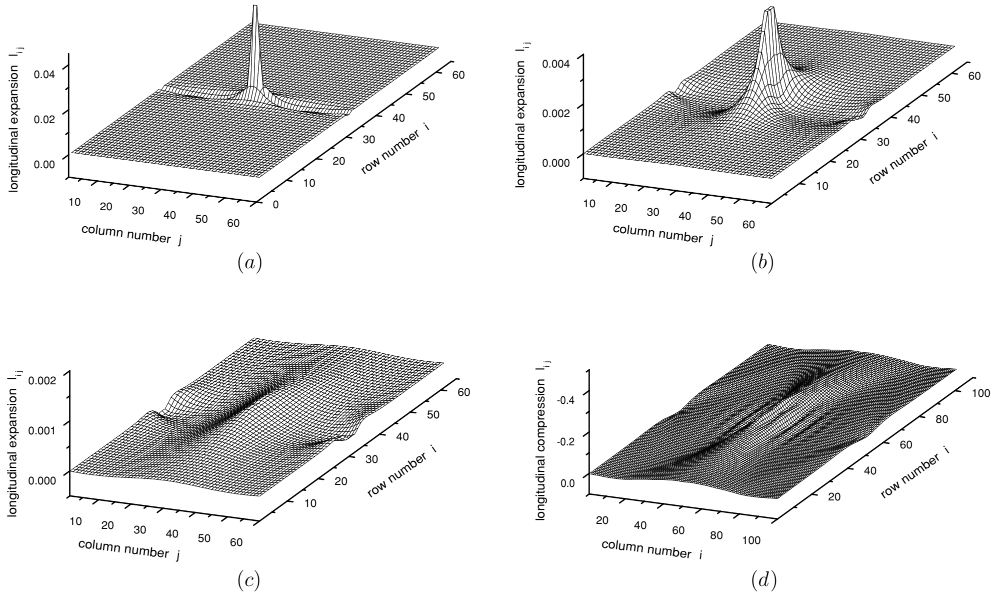

Figure 3. The results of solitary wave searching by numerical solving (26). The potential $\{c_1, c_2, c_3, c_4\}$ and soliton p_1 (see (4) and (5)) parameters are the same as in figure 2: $c_1 = 1.0$, $c_2 = 10.0$, $c_3 = 0.01$, $c_4 = 0.5$, $p_1 = 0.8$ (*a*); $c_1 = 1.0$, $c_2 = 10.0$, $c_3 = 0.02$, $c_4 = 0.1$, $p_1 = 0.8$ (*b*); $c_1 = 1.0$, $c_2 = 10.0$, $c_3 = 0.05$, $c_4 = 0.1$, $p_1 = 0.8$ (*c*); $c_1 = 1.0$, $c_2 = 0.0$, $c_3 = 0.5$, $c_4 = 0.5$, $p_1 = 0.3$ (*d*). In all cases, the soliton is centred in the geometrical centre of the lattice and solitons move along the rows.

One can see an essential difference in profiles for the last three cases (compare figures 2(*a*)–(*c*) and figures 3(*a*)–(*c*)). We attribute this fact to the analytical inaccuracy because of many approximations, and believe that the numerical solutions give more accurate results. As expected, both methods give coinciding soliton profiles (compare figures 2(*a*) and 3(*a*)) for the first parameters set (smallest c_3 and largest c_4 values). The final analysis of solitons stability is performed by molecular dynamics in the next section.

4. Soliton evolution on the 2D discrete lattice

In this section, we present the results on the solitons evolution and stability by molecular dynamics (MD) simulation. There are few commonly accepted approaches to prove the soliton stability. One approach is to follow a rather long trajectory with the initial condition in the form of assumed soliton solution. This method requires a large-scale MD simulation for 2D lattices, and our facilities do not allow to make it. Instead we utilize two other methods: (1) investigation of the solitons collision and (2) interaction of solitons with boundaries. The preserving of soliton shape after collision is expected in the first method. In the latter method, different solitons behaviour should occur after interaction with fixed and free boundaries. Namely, solitons survive after reflection at the fixed boundary and get destroyed after reflection at the free boundary.

Making transformation back to $\{x, y; t\}$ variables we get an expression for the analytical profile of the one-soliton solution,

$$u_x(x, y; t) = 4q_2 \frac{-\left[x - g_x - \left(c + \frac{q_1}{q_3}\rho^2\right)t\right]^2 + q_1^2\rho^2(y - g_y)^2 + 3\left(\frac{q_1}{\rho}\right)^2}{\left\{\left[x - g_x - \left(c + \frac{q_1}{q_3}\rho^2\right)t\right]^2 + q_1^2\rho^2(y - g_y)^2 + 3\left(\frac{q_1}{\rho}\right)^2\right\}^2}. \tag{29}$$

Here ρ, g_x and g_y are real soliton parameters (compare with complex parameters p_k, θ_k in (5)). ρ defines the soliton profile and velocity. The larger is ρ, the higher and more narrow is the soliton. The soliton velocity is given by (28) for $p_1 = \rho$ and (22) gives that $q_1/q_3 < 0$. Thus, $|v_{\mathrm{sol}}| < c$, i.e. solitons are subsonic, and the larger is the soliton amplitude, the slower is its velocity.

As was discussed earlier, for anharmonic terms U_1 in (7) one gets $k_1 > 0, k_2 < 0, k_3 < 0, k_4 > 0$, what results in $q_2 > 0$. So the amplitude of the excitation (29) is positive. Parameters g_x and g_y in (29) determine x and y coordinates of the soliton centre at $t = 0$, respectively.

The value u_x in (29) can be interpreted as a deformation of the lattice along the x-axis, i.e. deviation from the equilibrium distance between two nearest particles in one row $l_{ij} = u_{ij+1} - u_{ij}$. Positive value of u_x means the longitudinal expansion excitation.

Thus, in the case of the anharmonic NN interaction, soliton in 2D lattice is a localized expansion excitation travelling with subsonic velocity. Nonlinear character of (19) does not allow to change the sign of solution (29) ($u_x \to -u_x$). In other words, no stable nonlinear longitudinal compression excitations exist.

This fact provides a useful tool in MD simulations to check whether the excitation is soliton or not. If the excitation gets destroyed as a result of reversal of the sign of its amplitude, it is an evidence of a true soliton.

Later in this section, we present the results of MD simulations of the soliton evolution on the lattice with following parameters' values: $c_1 = 1.0, c_2 = 10.0, c_3 = 0.01, c_4 = 0.5$. Soliton profiles for these parameters are shown in figures 2(a) and 3(a).

The MD step is equal to 0.01, and the equations of motion were integrated by sixth-order predictor–corrector Gear algorithm [27]. Free boundary conditions are used. The advantage of this choice is the following. The reflection from free lattice boundaries changes the sign of an excitation amplitude, i.e. an expansion excitation transforms into a compression excitation and vice versa, which allows us to test the soliton nature of the excitation.

The square lattices up to 500×500 particles were considered. We use the fraction of 101×101 particles for better presentation later. Solitons are initially centred at the central row of the lattice, i.e. at the 51st row. For better viewing we cut the lattice along the central 51st row and show only half of the lattice from 51st to 101th rows. The omitted part of the lattice is the mirror reflection of what is shown.

First, we analyse the soliton evolution where the initial configuration is given by (29). Initial parameters are $\rho = 0.8, g_x = 10, g_y = 51$. Figure 4 demonstrates four snapshots of the soliton profile evolution at times $t_1 = 0, t_2 = 4 \times 10^4, t_3 = 9 \times 10^4$ and $t_4 = 11 \times 10^4$ MD steps.

One can see that the soliton travels with small loss of energy. The irradiated energy propagates in front of the soliton as its velocity is subsonic.

At t_3 the soliton reaches the right boundary of the lattice (see figure 4(c)) and reflects. The reflection at the free boundary causes the change of the amplitude sign and soliton transforms into compression excitation which is unstable, as discussed earlier (see figure 4(d)). This is an evidence of true soliton nature of the considered excitations.

Another essential feature of solitons worth mentioning is their stability in collision. Figure 5 illustrates the collision of two solitons. Initially at $t_1 = 0$ (figure 5(a)) two solitons are formed at the opposite ends of the lattice and move towards each other (figure 5(b), $t_2 = 3 \times 10^4$ MD steps). At $t_3 = 4 \times 10^4$ MD steps the solitons collide (figure 5(c)). Then, the solitons separate moving away from each other (figure 5(d), $t_4 = 4 \times 10^4$ MD steps). Figure 5(e) shows the moment when the solitons reach the opposite edges of the lattice at $t_5 = 7 \times 10^4$ MD steps. The initial soliton parameters are $\rho_1 = 0.8, g_{x1} = 15$ (left soliton),

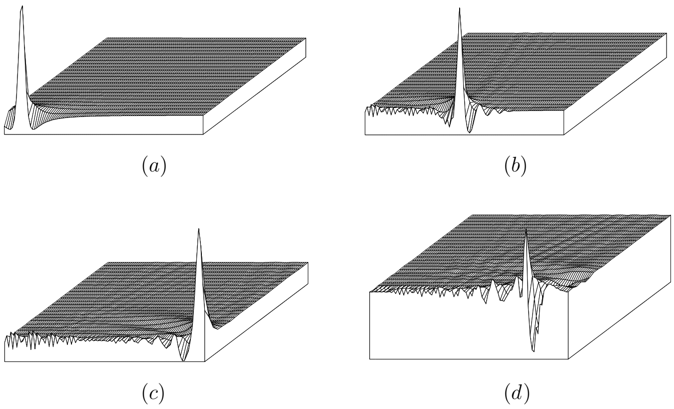

Figure 4. The results of the MD simulation of single soliton evolution on 101 × 101 lattice with parameters $c_1 = 1.0, c_2 = 10.0, c_3 = 0.01, c_4 = 0.5$. The initial soliton parameters are $\rho = 0.8$, $g_x = 10, g_y = 51$. The snapshots are made at times $t_1 = 0$ (*a*), $t_2 = 4 \times 10^4$ (*b*), $t_3 = 9 \times 10^4$ (*c*) and $t_4 = 11 \times 10^4$ (*d*) MD steps.

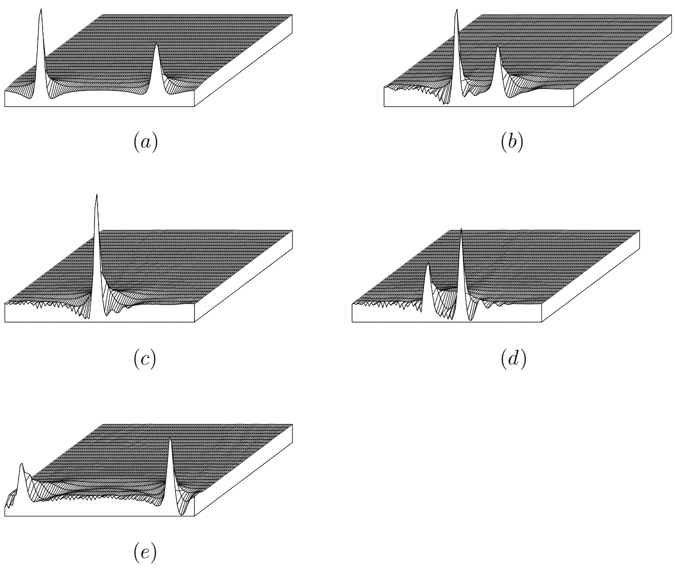

Figure 5. The results of the MD simulation of two solitons collision on 101 × 101 lattice with parameters $c_1 = 1.0, c_2 = 10.0, c_3 = 0.01, c_4 = 0.5$. The initial soliton parameters are $\rho_1 = 0.8, g_{x1} = 15, g_{y1} = 51, \rho_2 = 0.6, g_{x2} = 85, g_{y2} = 51$. The snapshots are made at times $t_1 = 0$ (*a*), $t_2 = 2 \times 10^4$ (*b*), $t_3 = 3 \times 10^4$ (*c*), $t_4 = 4 \times 10^4$ (*d*) and $t_5 = 7 \times 10^4$ (*e*) MD steps.

and $\rho_2 = 0.6$, $g_{x2} = 85$ (right soliton); $g_{y1} = g_{y2} = 51$. Some emission of energy is due to the discreetness of the lattice and high lattice deformation at the solitons collision. The general picture of two-soliton collision (figure 5) is very similar to those obtained for interaction between solitary waves in other 2D systems [12, 17].

Figure 6 demonstrates the solitons generation from some initial excitation. This excitation (see figure 6(*a*)) has a smooth localized profile of deformations and velocities in the

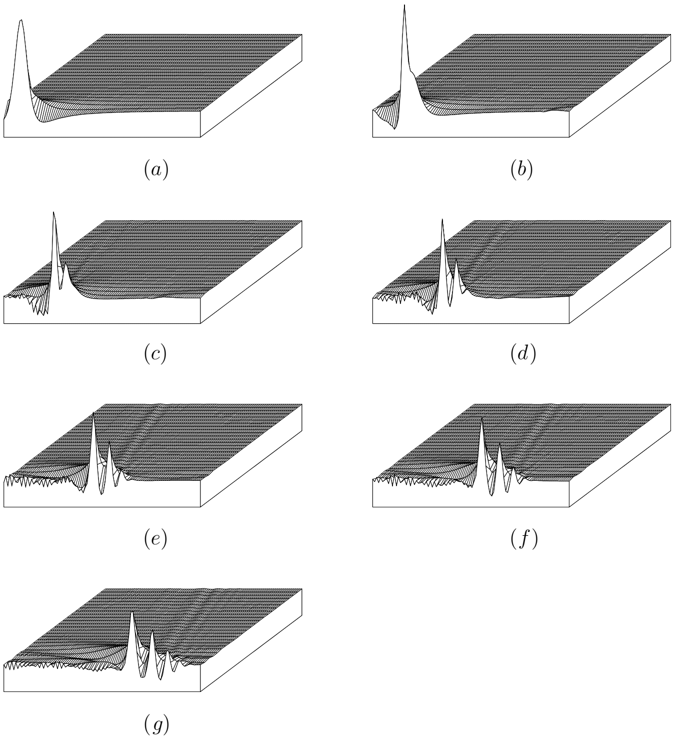

Figure 6. The separation of a set of solitons from initial smooth excitation on 101 × 101 lattice with parameters $c_1 = 1.0, c_2 = 10.0, c_3 = 0.01, c_4 = 0.5$. The initial excitation is centred at the 10th column and 51st row. The snapshots are made at times $t_1 = 0$ (*a*), $t_2 = 1 \times 10^4$ (*b*), $t_3 = 2 \times 10^4$ (*c*), $t_4 = 3 \times 10^4$ (*d*), $t_5 = 4 \times 10^4$ (*e*), $t_6 = 5 \times 10^4$ (*f*), and $t_7 = 6 \times 10^4$ (*g*) MD steps.

x-direction[1]. The initial excitation, after travelling some distance, splits into a set of well-distinguished solitons with different amplitudes and velocities. Since solitons considered here have subsonic velocities, one can expect the solitons generation behind the excitation front.

Figures 6(*b*)–(*g*) show solitons appearance one after another. In figure 6(*g*), four distinct solitons are finally separated. They are organized reversely to their amplitudes: soliton with the largest amplitude has the lowest velocity and the least width (leftmost soliton) as predicted (see (28)). The picture of solitons generation and separation from a certain initial condition is not a unique property of the considered system. This is a general property of the exactly solvable systems. And the picture of solitons separation demonstrated in figure 6 is similar to those observed in other 2D systems in [26].

Thus, one can conclude that solitons are characteristic excitations of the considered 2D nonlinear lattice and they can be generated by initial elongation excitation of a small part of the lattice. Numerical analysis shows that the number of solitons and their characteristics depend on the coordinates–velocities profile of the initial excitation.

As to the evolution of solitons with the other parameters shown in figures 2(*b*)–(*d*), the results of MD simulation are in good agreement with prediction of numerical PSM. Soliton from figure 2(*b*) is found to be rather stable. It evolves with slow decrease of the amplitude,

[1] The form of initial excitation is not essential. It should have an arbitrary localized expansion profile with momentum in the x-direction.

and the energy loss is a little larger than in the case of the soliton evolution from figure 2(*a*). Solitons from figures 2(*c*) and (*d*) are found to be unstable.

5. Conclusions

The main goal of the present paper was to analyse the nonlinear 2D lattice, to derive the KPI equation in the continuum approximation, to get the soliton solution and to determine the parameters range where this solution exists and is stable.

At least three types of interactions should be taken into account to ensure an existence of solitons. The first is the α-FPU-like NN interaction (U_1 in (7)). The next is the harmonic diagonal interaction (U_2 in (7)) ensuring mixing of x and y degrees of freedom and, as a consequence, soliton localization in both directions. And the third is the three-body interaction (U_3 in (7)). Symmetry of the potential prescribes also the symmetry of soliton propagation on the lattice: it can travel along symmetry axes of the square lattice with the coincidence of the total momentum and particles displacement from their equilibrium positions.

Two methods were utilized to get the soliton solution. The first is the analytical reductive perturbation method (RPM) which envisages many assumptions by going to continuum approximation and deriving final KP equation. RPM has limited level of accuracy and some doubts are cast upon the existence and stability of obtained solution. This issue is partially solved by the numerical pseudo-spectral method where the self-consistent determination of the soliton profile is based on Newtonian equations of motion. The PSM allows to refine the range of soliton parameters where the solution is stable.

But the final decision on the soliton stability was obtained in MD simulations. Two methods were utilized to convince the soliton stability: (1) collision of two solitons and (2) solitons interaction with boundaries. The preserving of solitons profiles after collision is an evidence for the true soliton nature of initial excitations.

The solutions of KP equations are the elongation solitons and no stable solutions for compression solitons exist. The reflection at free boundaries courses the change of the amplitude sign and as a result the soliton gets destroyed. In contrast, solitons survive after reflection at fixed boundaries. This fact is used to prove the soliton nature of the considered excitations.

Additionally, it was demonstrated that sets of subsonic solitons can be generated from the initial excitations (lattice deformation and total momentum) of an arbitrary bell-shaped excitation, the solitons number and their parameters being determined by the particular profile of an excitation.

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