



## Transverse instability of nonlinear longitudinal waves in hexagonal lattices

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Received 8 December 2014, accepted 20 May 2015, available online 28 August 2015

**Abstract.** Various continuum limits of the original discrete hexagonal lattice model are used to obtain transverse weakly nonlinear equations for longitudinal waves. It is shown, that the long wavelength continuum limit gives rise to the Kadomtsev–Petviashvili equation, while another continuum limit results in obtaining two-dimensional generalization of the nonlinear Schrödinger equation.

**Key words:** nonlinear hexagonal lattice, continuum limit, nonlinear differential equation, asymptotic solution.

### 1. INTRODUCTION

Nonlinear waves in crystals are studied using both discrete and continuum modelling [1–3]. However, while in the linear case both discrete and continuum equations may be analysed analytically, only a few discrete nonlinear equations are solved. Therefore, an approach, based on the continuum limit of the original discrete model, seems to be preferable. An important problem on this way is obtaining a correct continuum limit [3].

Recently, a two-dimensional (2D) weakly nonlinear hexagonal lattice model has been studied [4]. However, only plane longitudinal waves were considered. Nevertheless, it was found that dispersion relation for the discrete equations of the plane waves contains additional extrema in comparison with that of the 1D lattice model. It results in obtaining not only one- and two-field but also four-field continuum limits, which are valid for different intervals of the wavelengths. As a result, various nonlinear governing equations are obtained for all three cases, that possess nonlinear localized wave solutions or solitary wave solutions.

In this paper, the attention is paid to the modelling of a weak transverse instability of longitudinal plane waves in a hexagonal lattice. The linearized discrete equations are used to define a small parameter, responsible for the weak transverse effect while dispersion relation has the same form as for the plane waves. Only two of the three continuum limits are analysed. It results in the development of various nonlinear continuum models using different procedures of continualization. In particular, it allows us to find out how famous Kadomtsev–Petviashvili equation and 2D generalization of the nonlinear Schrödinger equation appear for the continuum description of nonlinear waves in the hexagonal lattice.

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## 2. STATEMENT OF THE PROBLEM

The hexagonal model considered represents a discrete structure, consisting of particles with equal masses  $M$ . Each particle is assumed to interact with six neighbouring particles, placed at equal distances  $l$ . The interaction forces are modelled by springs with linear rigidity,  $C$ , and nonlinear rigidity,  $Q$  (may be of either sign),

$$\Pi = \frac{1}{2}C \sum_i^6 \Delta l_i^2 + \frac{1}{3}Q \sum_i^6 \Delta l_i^3.$$

The expressions for elongations and the sketch of the structure are not presented here due to the lack of space. They may be found in [4]. The two-dimensional nonlinear discrete equations are obtained for horizontal ( $x_{m,n}$ ) and vertical ( $y_{m,n}$ ) displacements of a particle with numbers  $m, n$ , where  $m$  counts in horizontal direction. Using conventional expression for the kinetic energy, the Lagrangian is composed, and the Hamilton–Ostrogradsky variational principle is applied, resulting in

$$\begin{aligned} M(x_{m,n})_{tt} + \frac{1}{4}C & ((x_{m,n} - x_{m-1,n-1}) + (x_{m,n} - x_{m-1,n+1}) + (x_{m,n} - x_{m+1,n-1}) \\ & + (x_{m,n} - x_{m+1,n+1}) - 4(x_{m-2,n} + x_{m+2,n} - 2x_{m,n})) \\ + \frac{\sqrt{3}}{4} C & ((y_{m,n} - y_{m-1,n-1}) + (y_{m,n} - y_{m+1,n+1}) + (y_{m-1,n+1} - y_{m,n}) + (y_{m+1,n-1} - y_{m,n})) \\ + \frac{1}{8}Q & ((x_{m,n} - x_{m-1,n-1})^2 + (x_{m,n} - x_{m-1,n+1})^2 - (x_{m,n} - x_{m+1,n-1})^2 \\ & - (x_{m,n} - x_{m+1,n+1})^2 + 8[(x_{m,n} - x_{m-2,n})^2 - (x_{m,n} - x_{m+2,n})^2]) \\ + \frac{\sqrt{3}}{4}Q & ((x_{m,n} - x_{m-1,n-1})(y_{m,n} - y_{m-1,n-1}) - (x_{m,n} - x_{m-1,n+1})(y_{m,n} - y_{m-1,n+1}) \\ & + (x_{m,n} - x_{m+1,n-1})(y_{m,n} - y_{m+1,n-1}) - (x_{m,n} - x_{m+1,n+1})(y_{m,n} - y_{m+1,n+1})) \\ + \frac{3}{8}Q & ((y_{m,n} - y_{m-1,n-1})^2 + (y_{m,n} - y_{m-1,n+1})^2 - (y_{m,n} - y_{m+1,n-1})^2 - (y_{m,n} - y_{m+1,n+1})^2) = 0, \quad (1) \end{aligned}$$

$$\begin{aligned} M(y_{m,n})_{tt} + \frac{\sqrt{3}}{4}C & ((x_{m,n} - x_{m-1,n-1}) + (x_{m,n} - x_{m+1,n+1}) + (x_{m-1,n+1} - x_{m,n}) + (x_{m+1,n-1} - x_{m,n})) \\ + \sqrt{3} & [(y_{m,n} - y_{m-1,n-1}) + (y_{m,n} - y_{m-1,n+1}) + (y_{m,n} - y_{m+1,n-1}) + (y_{m,n} - y_{m+1,n+1})] \\ + \frac{1}{8}Q & (\sqrt{3} [(x_{m,n} - x_{m-1,n-1})^2 - (x_{m,n} - x_{m-1,n+1})^2 + (x_{m,n} - x_{m+1,n-1})^2 - (x_{m,n} - x_{m+1,n+1})^2]) \\ + 6 & [(x_{m,n} - x_{m-1,n-1})(y_{m,n} - y_{m-1,n-1}) + (x_{m,n} - x_{m-1,n+1})(y_{m,n} - y_{m-1,n+1}) \\ & - (x_{m,n} - x_{m+1,n-1})(y_{m,n} - y_{m+1,n-1}) - (x_{m,n} - x_{m+1,n+1})(y_{m,n} - y_{m+1,n+1})] \\ + 3\sqrt{3} & [(y_{m,n} - y_{m-1,n-1})^2 - (y_{m,n} - y_{m-1,n+1})^2 + (y_{m,n} - y_{m+1,n-1})^2 - (y_{m,n} - y_{m+1,n+1})^2] = 0. \quad (2) \end{aligned}$$

Only longitudinal plane waves,  $x_m$ , propagation along the  $x$  axis were considered in [4]. For this purpose, it was assumed that  $y_{m,n} = 0$  and no variations with respect to  $n$  happen in Eqs (1) and (2). Now the attention is paid to the influence of transverse variations. For this purpose, first, the linearized equations are studied.

### 3. LINEAR ANALYSIS

The linearized governing equations for  $Q = 0$  are

$$\begin{aligned}
 M(x_{m,n})_{tt} + \frac{1}{4}C((x_{m,n} - x_{m-1,n-1}) + (x_{m,n} - x_{m-1,n+1}) + (x_{m,n} - x_{m+1,n-1}) \\
 + (x_{m,n} - x_{m+1,n+1}) - 4(x_{m-2,n} + x_{m+2,n} - 2x_{m,n})) \\
 + \frac{\sqrt{3}}{4}C((y_{m,n} - y_{m-1,n-1}) + (y_{m,n} - y_{m+1,n+1}) + (y_{m-1,n+1} - y_{m,n}) + (y_{m+1,n-1} - y_{m,n})) = 0, \quad (3)
 \end{aligned}$$

$$\begin{aligned}
 M(y_{m,n})_{tt} + \frac{\sqrt{3}}{4}C((x_{m,n} - x_{m-1,n-1}) + (x_{m,n} - x_{m+1,n+1}) + (x_{m-1,n+1} - x_{m,n}) + (x_{m+1,n-1} - x_{m,n}) \\
 \sqrt{3}[(y_{m,n} - y_{m-1,n-1}) + (y_{m,n} - y_{m-1,n+1}) + (y_{m,n} - y_{m+1,n-1}) + (y_{m,n} - y_{m+1,n+1})]) = 0. \quad (4)
 \end{aligned}$$

The dispersion relation is obtained after presenting the solutions in the form

$$x_{m,n} = A \exp(i(k_x l_x m + k_y l_y n - \omega t)), \quad y_{m,n} = B \exp(i(k_x l_x m + k_y l_y n - \omega t)), \quad (5)$$

where  $l_x = l/2, l_y = \sqrt{3} l/2$ . Let us consider only the case of weak transverse variations along the vertical axis  $y, k_y l_y = \varepsilon \bar{k}_y l_y$ . Then one obtains  $\cos k_y l_y \approx 1, \sin k_y l_y \approx \varepsilon \bar{k}_y l_y$ . The substitution of Eq. (5) into Eqs (3) and (4) results in

$$A \left( \frac{2M}{C} \omega^2 - 6 + 2 \cos(k_x l_x) + 4 \cos(2k_x l_x) \right) - 2\sqrt{3} \varepsilon B \bar{k}_y l_y \sin(k_x l_x) = 0, \quad (6)$$

$$\sqrt{3} \varepsilon A \bar{k}_y l_y \sin(k_x l_x) - B \left( \frac{M}{C} \omega^2 - 3 + 3 \cos(k_x l_x) \right) = 0. \quad (7)$$

Equalization of orders in Eq. (7) implies an assumption  $B = \varepsilon \bar{B}$  that corresponds to a weak shear wave. Then Eq. (6) gives rise to the asymptotic expression of the dispersion relation

$$\omega^2 = \frac{2C}{M} \sin^2 \left( \frac{k_x l_x}{2} \right) \left( 9 - 8 \sin^2 \left( \frac{k_x l_x}{2} \right) \right) + O(\varepsilon^2), \quad (8)$$

while Eq. (7) results in the relationship between  $A$  and  $B$ . The leading order part of the dispersion relation corresponds to the case of plane waves that was studied in detail in [4]. Three possibilities for continualization have been found there, here the two of them will be considered, namely, the solution at small wave numbers,  $k_x l_x \ll 1$ , that corresponds to the area near the origin at the dispersion curve, and the solution in the vicinity of  $k_x l_x = \pi$  that corresponds to the minimum of the dispersion curve [4]. In the last case, one can write  $k_x l_x = \pi + k_1 l_x$  and consider small values of  $k_1 l_x$ .

### 4. FIRST CONTINUUM LIMIT

An analysis of the linearized discrete equations allows us to obtain continuum equations for longitudinal waves propagating along horizontal  $x$  direction and weakly perturbed in vertical  $y$  direction. For this purpose, the continuum displacements of the central particle,  $x_{m,n}, y_{m,n}$ , are  $u(x, Y, t), \varepsilon v(x, Y, t)$  respectively where  $Y = \varepsilon y, \varepsilon \ll 1$  is a small parameter. Then the Taylor series for neighbouring particles may be written as

$$x_{m\pm 1, n\pm 1} = u \pm l_x u_x \pm \varepsilon l_y u_Y + \frac{1}{2} l_x^2 u_{xx} + \varepsilon l_x l_y u_{xY} + \frac{1}{2} \varepsilon^2 l_y^2 u_{YY} + \dots$$

The additional scaling is needed to characterize orders of nonlinear and higher-order derivative linear terms (dispersion) besides weak transverse variations (diffraction). Let us introduce  $T^*$  as a scale for time,  $L$  as a scale for  $x$  and  $A$  as a scale for the displacements  $u$  and  $v$ . Note that the dimension of  $Q$  differs from that of  $C$ , then one assumes that  $Q = \bar{Q}/l$ . One assumes that  $T^* = L/c$  where  $c$  is the velocity of linear longitudinal waves,  $c = \sqrt{9C l^2/(8M)}$ . Equal orders of nonlinear and dispersion terms require  $A = \delta^2$ ,  $l/L = \delta$ , where  $\delta$  is a small parameter. One assumes also that  $\delta \sim \varepsilon$  to get equal contribution of nonlinear, dispersive and diffraction terms that correspond to the most interesting case.

Substituting the Taylor series into the discrete governing equations (1) and (2) and omitting bars in notations for nondimensional variables for simplicity, one obtains

$$u_{tt} - u_{xx} - \varepsilon^2 \left( \frac{2}{3} v_{xY} + \frac{1}{3} u_{YY} + \frac{11Q}{6} u_x u_{xx} + \frac{11}{144} u_{xxxx} \right) = O(\varepsilon^3), \quad (9)$$

$$v_{tt} - \frac{1}{3} v_{xx} - \frac{2}{3} u_{xY} = O(\varepsilon). \quad (10)$$

Equations (9) and (10) may be uncoupled when a solution is considered that depends on the phase variable  $\xi = x - t$ , vertical coordinate  $Y$  and slow time  $\tau = \varepsilon^2 t$ ,  $u = u(\xi, Y, \tau)$ ,  $v = v(\xi, Y, \tau)$ . Then Eq. (10) is resolved for  $v_\xi$ ,

$$v_\xi = u_Y,$$

while Eq. (9) becomes the well-known Kadomtsev–Petviashvili equation for the longitudinal strain  $w = u_\xi$ ,

$$\left( 2w_\tau + \frac{11Q}{6} w w_\xi + \frac{11}{144} w_{\xi\xi\xi} \right)_\xi + w_{YY} = 0. \quad (11)$$

The signs at the coefficients of the equation correspond to the case of transverse stability of the plane waves [5]. Two-dimensional localized structures are accounted for the exact two-soliton solution [5]. Detailed analysis of this solution may be found in [6,7]. Also numerical simulations of initially non-interacting plane waves reveals abnormal increase in the amplitude in the area of the waves interaction [7,8].

## 5. SECOND CONTINUUM LIMIT

One cannot apply the same continualization procedure for small  $k_1 l_x$  [3,4]. One has to introduce before the displacements of even and odd particles,  $p_{1m,n}$ , and  $p_{2m,n}$  for the horizontal displacement,  $x_{m,n}$ , and  $q_{1m,n}$ , and  $q_{2m,n}$  for the vertical displacement,  $y_{m,n}$ . Since displacements of even and odd lie each at its smooth curve (see [4]), now the procedure of continualization from the previous section may be applied to them separately. It results in obtaining four continuum equations for the continuum displacements  $u_1(x, Y, t)$ ,  $\varepsilon v_1(x, Y, t)$  chosen for the even central particle  $p_{1m,n}$ ,  $q_{1m,n}$ , and for the functions  $u_2(x, Y, t)$ ,  $\varepsilon v_2(x, Y, t)$ , describing continuum displacements of the odd particle,  $p_{2m,n}$ ,  $q_{2m,n}$ .

Displacements of even and odd masses cannot be recognized in the continuum description. Therefore new variable are more reasonable for the continuum description,

$$U_1 = \frac{u_1 + u_2}{2}, \quad U_2 = \frac{u_1 - u_2}{2}, \quad V_1 = \frac{v_1 + v_2}{2}, \quad V_2 = \frac{v_1 - v_2}{2}.$$

New variables  $U_1, V_1$  account for conventional macro-displacements, while the variables  $U_2, V_2$  describe the influence of the internal structure. The governing equations in new variables are written omitting negligibly small terms (that will be seen from the forthcoming solution),

$$MU_{1,tt} - \frac{9C l^2}{8} U_{1,xx} - Q I U_2 U_{2,x} = 0, \quad (12)$$

$$MV_{1,tt} - \frac{3Cl^2}{8}V_{1,xx} - \frac{3Cl^2}{4}U_{1,xY} = 0, \tag{13}$$

$$MU_{2,tt} + 2CU_2 + 2 - \frac{7Cl^2}{8}U_{2,xx} + Ql_xU_2U_{1,x} + \frac{3\varepsilon^2Cl^2}{8}(2V_{2,xY} + U_{2,YY}) = 0, \tag{14}$$

$$MV_{2,tt} + 6CV_2 + \frac{3Cl^2}{8}V_{2,xx} + \frac{3Cl^2}{4}U_{2,xY} = 0. \tag{15}$$

Let us assume that

$$U_2 = \varepsilon U_{21} + \varepsilon^2 U_{22} + \varepsilon^3 U_{23} + \dots \tag{16}$$

Substituting the series into Eq. (14) and equating to zero terms at each order of  $\varepsilon$ , one obtains that equation at the leading order  $\varepsilon$  is

$$MU_{21,tt} + 6CU_{21} + \frac{3Cl^2}{8}U_{21,xx} = 0. \tag{17}$$

The solution of Eq. (17) is

$$U_{21} = B(X, T, \tau) \exp(i\theta) + B^*(X, T, \tau) \exp(-i\theta),$$

where

$$\theta = kx - \omega t, X = \varepsilon x, T = \varepsilon t, \tau = \varepsilon^2 t,$$

and

$$\omega^2 = \frac{2C}{M} + \frac{7Cl^2k^2}{8M}. \tag{18}$$

Then the solution for  $U_{1,\theta}$  is obtained from Eq. (12),

$$U_{1,\theta} = \frac{2\varepsilon^2 Ql}{C(8 - l^2k^2)} (B^2 \exp(2i\theta) + B^{*2} \exp(-2i\theta)), \tag{19}$$

while the solution for  $V_2$  is obtained from Eq. (15)

$$V_2 = -\frac{3i\varepsilon kl^2}{16 - 5l^2k^2} (B_Y \exp(i\theta) - B_Y^* \exp(-i\theta)). \tag{20}$$

Equation (14) at the next order  $\varepsilon^2$  is

$$MU_{22,tt} + 6CU_{22} + \frac{3Cl^2}{8}U_{22,xx} = i \left( 2M\omega B_T + \frac{7Cl^2}{4}kB_X \right) \exp(i\theta) - i \left( 2M\omega B_T^* + \frac{7Cl^2}{4}kB_X^* \right) \exp(-i\theta). \tag{21}$$

The r.h.s. in Eq. (21) gives rise to the secular terms in the solution for  $U_{22}$ . To avoid secular terms, one has to equate to zero coefficients at  $\exp(\pm i\theta)$  that results in an equation for  $B$ ,

$$2M\omega B_T - \frac{7Cl^2}{4}kB_X = 0.$$

It means that  $B = B(\zeta, \tau)$ , where

$$\zeta = X - \frac{7Cl^2k}{8M\omega}T. \tag{22}$$

Then the r.h.s. in Eq. (21) is zero that allows us to obtain the solution  $U_{22} = 0$ .

Substituting Eqs (19) and (20) into Eq. (21) at order  $\varepsilon^3$  one obtains that the absence of secular terms results in the equation for  $B$  in the form of the two-dimensional nonlinear Schrödinger equation

$$2i\omega_2 MB_\tau + \frac{7C^2l^2}{4M\omega^2} B_{\zeta\zeta} - \frac{3Cl^2(16 - 11l^2k^2)}{8(16 - 5l^2k^2)} B_{YY} - \frac{2Q^2l^2}{C(8 - l^2k^2)} B^2 B^* = 0. \tag{23}$$

This equation has been obtained and studied for the description of the deep water surface waves [5,9]. Certainly, the plane wave solution may be obtained where the sign of the product of the coefficients at nonlinear and dispersive terms defines the existence of either bright or dark solitons. Transverse instability of the plane solitary wave has been studied numerically in [9] and asymptotically in [10]. In the paper a large variety of the methods is employed and various kinds of instabilities revealed for bright and dark plane solitary waves.

The solution for  $V_1$  is obtained from Eq. (13) using the solution for  $U_2$ .

## 6. CONCLUSIONS

The solution for the plane longitudinal wave in a hexagonal lattice from [4] is extended by the case of weakly transverse variations. Use of two continuum limits allows us to obtain different model equations. Thus, the Kadomtsev–Petviashvili equation arises for the case of long wavelength while a two-dimensional generalization of the two-dimensional nonlinear Schrödinger equation appears when the short wavelength case is considered. The solution in the last case describes not only the macro-strain evolution but also internal variations in the structure of the material.

The fact that weakly transverse equations have the form of familiar equations allows us to study transverse instability of longitudinal strain waves using already known solutions [5,10]; in particular, making conclusions about transverse stability in the first long-wave continuum limit.

Only weakly nonlinear theory is considered in the paper. Recently, another form (through trigonometric functions) of nonlinear terms has been suggested to account for large strains in a one-dimensional diatomic lattice [11,12]. Similar generalization for a hexagonal lattice will be done in due time.

## ACKNOWLEDGEMENTS

The work of the first author has been partly supported by the Russian Foundation for Basic Researches (grant No. 12-01-00521-a) and by the DAAD Fellowship (grant A1400380).

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## Mittelineaarsete pikilainete ristsuunaline ebastabiilsus heksagonaalses võres

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Kristallides levivate mittelineaarsete lainete uurimisel kasutatakse nii pideva keskkonna teooriatel põhinevaid kui ka diskreetseid mudeleid. Algselt diskreetsest heksagonaalse võre mudelist pideva keskkonna teooriale vastavate ja nõrgalt ristsuunas levivaid pikilaineid kirjeldavate võrrandite tuletamiseks on kasutusel mitmeid pideva keskkonna piirteooriaid. Käesolevas artiklis on näidatud, et pika lainepikkuse piirteooria rakendamine annab tulemuseks Kadomtsevi-Petviashvili võrrandi, kuid lühikese lainepikkuse piirteooria rakendamise korral saadakse tulemuseks mittelineaarne kahemõõtmeline Schrödingeri võrrand.