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# Non-linear plane waves in materials having hexagonal internal structure

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ABSTRACT

Three different continuum limits for modeling non-linear plane waves in two-dimensional hexagonal lattice are obtained. New coupled non-linear continuum equations are obtained to study the interaction of a macro-strain wave and the waves caused by variations in an internal structure. New analytical solutions are obtained to describe localized non-linear strain waves. It is shown that the solutions are different from those of the 1D lattice model due to the inclusion of non-neighboring interactions in a lattice.



## 1. Introduction

An important problem is how to describe correctly an influence of an internal structure of a crystal on the description of dynamic strain processes in it. One possibility is in a correct continuum limit of a crystalline discrete model of a material. This approach may be more efficient than that based on an addition of the so-called gradient terms in the expression of internal or free energy of deformation within the framework of a pure continuum approach.

Starting from the one-dimensional (1D) lattice model of equal particles connected by cental springs [1–4], further studies developed into the lattices with additional degrees of freedom [5–10], lattices with particle interaction extending beyond nearest neighbors [11,12] and various two-dimensional (2D) lattices [6,7,13–18]. The hexagonal 2D lattice attracts considerable attention due to its use for the description of carbon nanotubes, graphene, etc. [14,15]. Usually the familiar acoustic continuum limit is used to obtain continuum equations [2,5,6,16,17]. However, even for the 1D lattice, another case was found in [3] that corresponds to the modeling of the coupling between the waves belonging to acoustic and optical branches of the dispersion relation. Further this idea was extended in [9,10] to develop the so-called two-, three- and four-field continuum models for lattices with additional degrees of freedom. It turns out that these extended models allow us to describe the waves behavior in various parts of the dispersion curve, not only near the axes origin for the acoustic branch.

Most of the works concern about linear description [2,7–11,16–18]. In this case an analysis of the discrete dispersion relation gives rise to the linear continuum equations of motion whose solution accounts for harmonic and pulse linear waves [16,18]. Some works consider only long wavelength (or acoustic) continualization [7,16–18] while other authors try to extend the modeling [9,10] by developing the multi-field approach. It allows them to include the higher-order gradient terms to the governing equations, thus, to describe a microstructure of a material. The solutions of the equations account for long- and short-wavelength strains.

Non-linear models [2,5,6,19,20] usually treat only long wave continualization. However, the two-field modeling equations for the 1D lattice were obtained in [3,4]. Similarly, recent study of di-atomic lattice in [21] resulted in obtaining two-field coupled non-linear equations.

In this paper, a 2D linear hexagonal lattice model studied in [16,17] is extended up to a weakly non-linear level. The 2D non-linear waves description is too complicated for an analysis. That is why we restricted our consideration by the plane waves only. It is found that dispersion relation for the discrete equations of the plane wave solutions contains additional extrema in comparison with the 1D lattice model. It allows us to suggest not only one- and two-field but also four-field continuum limits. The non-linear governing equations are obtained for all three cases, and their localized wave solutions are obtained and analyzed.

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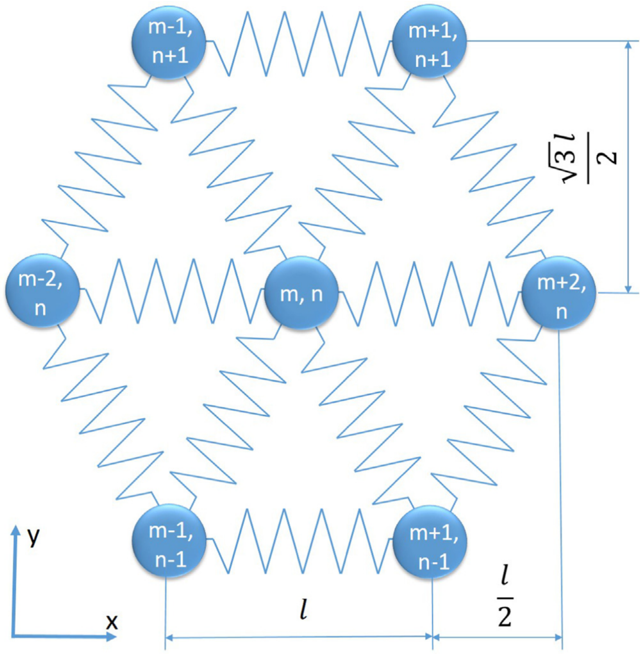


**Fig. 1.** Two-dimensional hexagonal lattice.

## 2. Statement of the problem

We consider a weak non-linear generalization of the hexagonal model studied in [16]. The discrete structure is shown in Fig. 1, it consists of the particles with equal masses $M$ placed at the equal relative distances $l$. Each particle is assumed to interact with six neighboring particles. The interaction forces are modeled by equal springs with linear rigidity $C$ and non-linear rigidity $Q$, the last may be of either sign. Then the kinetic energy is written similar to [16]

$$T_{m,n} = \frac{1}{2} M\left(\dot{x}_{m,n}^2 + \dot{y}_{m,n}^2\right),$$

while the potential energy of [16] is generalized by non-linear terms:

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

where $x_{m,n}$ and $y_{m,n}$ are respectively the horizontal and vertical displacements of particle $m, n$. The expressions for elongations of the springs, $\Delta l_i$, are

$$\Delta l_1 = x_{m+2,n} - x_{m,n}$$

$$\Delta l_2 = \frac{1}{2}(x_{m+1,n+1} - x_{m,n} + \sqrt{3}[y_{m+1,n+1} - y_{m,n}])$$

$$\Delta l_3 = \frac{1}{2}(x_{m,n} - x_{m-1,n+1} + \sqrt{3}[y_{m-1,n+1} - y_{m,n}])$$

$$\Delta l_4 = x_{m,n} - x_{m-2,n}$$

$$\Delta l_5 = \frac{1}{2}(x_{m,n} - x_{m-1,n-1} + \sqrt{3}[y_{m,n} - y_{m-1,n-1}])$$

$$\Delta l_6 = \frac{1}{2}(x_{m+1,n-1} - x_{m,n} + \sqrt{3}[y_{m,n} - y_{m+1,n-1}])$$

where the springs are numbered counter-clockwise.

Then the Lagrangian may be composed, and the Hamilton–Ostrogradsky variational principle is applied to obtain the governing equations in the form

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

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

The linear part of the equations coincides with the equations of motion from Ref. [16].

## 3. Plane waves: linear analysis

An analysis of non-linear difference equations (1) and (2) is rather difficult. That is why we begin with consideration of longitudinal plane waves. For this purpose, assume that $y_{m,n} = 0$ and no variations with respect to $n$ happen in Eqs. (1) and (2). It corresponds to the consideration of plane wave $x_m$ along the $x$-axis. Then Eq. (2) is satisfied identically while Eq. (1) is

$$\begin{aligned}
M(x_m)_{tt} = {} & C(x_{m+2} - 3x_m + 0.5x_{m+1} + 0.5x_{m-1} + x_{m-2}) \\
& + Q\left((x_{m+2} - x_m)^2 - \frac{1}{4}(x_m - x_{m-1})^2\right. \\
& \left. + \frac{1}{4}(x_{m+1} - x_m)^2 - (x_m - x_{m-2})^2\right).
\end{aligned} \tag{3}$$

Different from the familiar 1D lattice, now the equation describes also non-neighboring interactions similar to the model considered in [11]. The role of these interactions may be clarified by considering the linearized version of Eq. (3) at $Q = 0$.

The solution of the linearized Eq. (3) is sought as $x_m = A\exp(\imath(km - \omega t))$, $k = k_x l_x$, $l_x = l/2$. Then the dispersion relation is

$$\omega^2 = \frac{2C}{M}\sin^2(k/2)(9 - 8\sin^2(k/2)). \tag{4}$$

One can note the last term in brackets in Eq. (4) that is absent in the dispersion relation for the 1D lattice with equal particles