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OPERATOR APPROACH TO SQUARE LATTICE NONLINEAR DYNAMICS

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Abstract. Two dimensional square lattice is considered when the forces between the lattice particles are expressed both linearly and quadratically dependent on the spring elongations. The shift operator approach, firstly developed by [1] and applied to the one-dimensional linear problem, is extended on the two-dimensional nonlinear case. The discrete strain energy and the discrete governing nonlinear equations of motion are obtained. Also, the continuum nonlinear equation for the plane longitudinal waves propagation is obtained in a weakly nonlinear case.
Keywords: lattice; nonlinear modeling; strain wave.

1. Introduction

One of the most important contributions done by Eron Aero and Gerard Maugin concerns dynamical processes in nonlinear lattices [2,3,4,5]. The first success in describing materials' internal structure by means of modelling with different types of lattices is connected with the name of M. Born, who presented and solved the wave propagation problem in a one-dimensional chain [6]. Recent achievements may be found, e.g., in Refs. [2,3,7,8]. The problem of linear waves propagation in the one-dimensional monoatomic chain, where particles are represented by the material points with a nonzero mass, and the interatomic bonds are described by elastic springs, has become classical [7,8,9]. The importance of nonlinear interactions has risen after the investigation of Fermi, Pasta and Ulam in 1955 [10], which presented the model of one-dimensional string of nonlinearly interacting particles that did not show energy equipartition, i.e. practically the entire energy was concentrated in the first mode, and thus, nonlinearity doesn't guarantee the energy transfer of the long-wavelength oscillations into the equilibrium distribution.

Since then, the field has been widely developed by different scientists [11], such as Sievers and Takeno, Ovchinnikov, Kosevich and Kovalev [12-14], whose works brought into attention the subject of intrinsic localized modes (or discrete breathers) in anharmonic lattices. This development has mainly been inspired by the experimental observation of nonlinear modes in a wide range of physical systems in mechanics [8,9,15], electronics [16,17], biophysics (formation of denaturation bubbles in the DNA double strand dynamics) [18], solid state physics, e.g.in [2] aspects of deformable solids (also known as inelastic crystals) nonlinear dynamics are considered, where nonlinear effects combine or compete with each other. Various models were investigated - both discrete and continuum, in particular, the effects of thermal, electric or magnetic nature in the crystal structure, and were analyzed utilizing the equations of

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rational mechanics. The nonlinear effects are also of great importance in atomic physics and nonlinear optics, emergence of dynamical instabilities, discrete quantum self-trapping and localized modes in the ultracold Bose-Einstein condensates in the presence of deep optical lattices, see e.g. [19], granular crystals, presence of solitary waves in granular crystals consisting of beads with the Hertzian elastic interactions [20] in addition to the latter achievements in material engineering [21].

The dynamic processes in crystals are considered using both continuum and discrete approaches. In the linear case, both approaches give rise to equations whose solutions are possible to find. Unlike that, only a few discrete nonlinear equations have analytical solutions, e.g. Toda lattice equations, or Ablowitz-Ladik equation. [22,23]. This is the reason for utilizing the continuum limit of the original discrete equation to obtain governing nonlinear equations. Derivation of governing equations often faces with complicated transformations, especially, in the multi-dimensional problems. Hence, there is a need in a compact procedure allowing us to obtain governing equations of motion. A promising procedure concerns utilization of the shift operators as shown in Ref. [1].

In this paper, the application of the shift-operator approach [1] is extended by the two-dimensional and nonlinear case in Sect. 1. The expression for the strain discrete energy is obtained and written in terms of the shift operators in Sect. 2. Then the nonlinear discrete equations of motion are obtained using the variational principle. The continuum equations are derived for longitudinal plane waves.

2. Statement of the problem and shift operator formalism

Consider a square lattice with particles of equal masses m, see Fig. 1. Let the interactions between particles are modeled by nonlinearly elastic springs. The linear rigidities are C_1 for horizontal and vertical interactions and C_2 for diagonal interactions. Similarly, nonlinear rigidities are introduced, Q_1 for horizontal and vertical interactions and Q_2 for diagonal interactions. The displacement vector for the particle with the number m,n is $\vec{U}_{m,n} = u_{m,n}\vec{i} + v_{m,n}\vec{j}$, where $u_{m,n}$ and $v_{m,n}$ are the horizontal and vertical components of the displacement vector respectively and $\vec{i}$ and $\vec{j}$ are the unit vectors in horizontal and vertical directions.

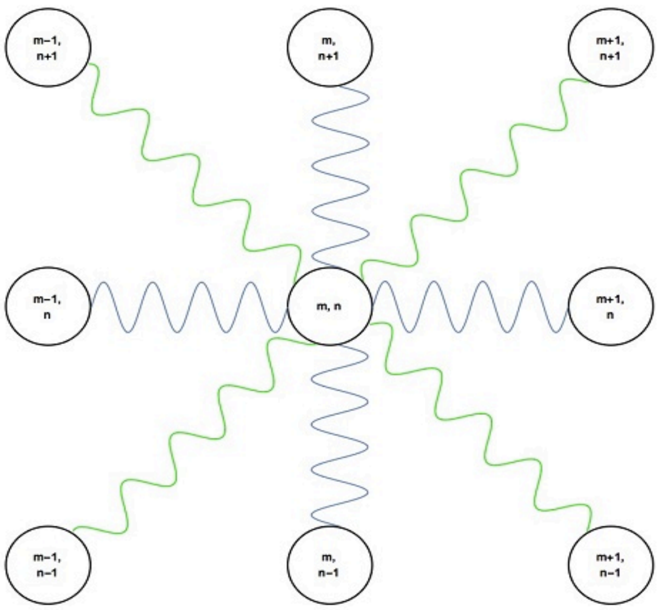

Fig.1. Square lattice model.

The shift operators,

$$D_1 = \sum_m \frac{h^m}{m!}\frac{d^m}{dx^m} = e^{h\frac{d}{dx}},$$

$$D_2 = \sum_n \frac{h^n}{n!}\frac{d^n}{dy^n} = e^{h\frac{d}{dy}},$$

$$D_1^\dagger = \sum_m \frac{-h^m}{m!}\frac{d^m}{dx^m} = e^{-h\frac{d}{dx}},$$

$$D_2^\dagger = \sum_n \frac{-h^n}{n!}\frac{d^n}{dy^n} = e^{-h\frac{d}{dy}},$$

$$D_1 * D_2 = \sum_{m,n}(\frac{h^m}{m!}\frac{d^m}{dx^m} + \frac{h^n}{n!}\frac{d^n}{dy^n}) = e^{h\frac{d}{dx}+h\frac{d}{dy}},$$

$$D_1 * D_2^\dagger = \sum_{n,m}(\frac{h^m}{m!}\frac{d^m}{dx^m} + \frac{-h^n}{n!}\frac{d^n}{dy^n}) = e^{h\frac{d}{dx}-h\frac{d}{dy}},$$

$$D_1^\dagger * D_2 = \sum_{n,m}(\frac{-h^m}{m!}\frac{d^m}{dx^m} + \frac{h^n}{n!}\frac{d^n}{dy^n}) = e^{-h\frac{d}{dx}+h\frac{d}{dy}},$$

$$D_1^\dagger * D_2^\dagger = (\sum_{n,m}\frac{-h^m}{m!}\frac{d^m}{dx^m} + \frac{-h^n}{n!}\frac{d^n}{dy^n}) = e^{-h\frac{d}{dx}-h\frac{d}{dy}},$$

act on the function $u(x_m,y_n)$ as:

$$\begin{aligned}
D_1 u_{m,n} &= u(x_m+h, y_n) = u(x_{m+1}, y_n) = u_{m+1,n},\\
D_1^\dagger u_{m,n} &= u(x_m-h, y_n) = u(x_{m-1}, y_n) = u_{m-1,n},\\
D_2 u_{m,n} &= u(x_m, y_n+h) = u(x_m, y_{n+1}) = u_{m,n+1},\\
D_2^\dagger u_{m,n} &= u(x_m, y_n-h) = u(x_m, y_{n-1}) = u_{m,n-1},\\
D_1 * D_2 u_{m,n} &= u(x_m+h, y_n+h) = u(x_{m+1}, y_{n+1}) = u_{m+1,n+1},\\
D_1 * D_2^\dagger u_{m,n} &= u(x_m+h, y_n-h) = u(x_{m+1}, y_{n-1}) = u_{m+1,n-1},\\
D_1^\dagger * D_2 u_{m,n} &= u(x_m-h, y_n+h) = u(x_{m-1}, y_{n+1}) = u_{m-1,n+1},\\
D_1^\dagger * D_2^\dagger u_{m,n} &= u(x_m-h, y_n-h) = u(x_{m-1}, y_{n-1}) = u_{m-1,n-1}.
\end{aligned} \tag{1}$$

Similar expressions hold for the action on the function $v(x_n,y_m)$.

The shift operators are used to model the interaction forces between particles in the lattice. To obtain the expressions for the forces correctly, we have to introduce the vectors $\vec{n}_j$, accounting for the direction from the particle m,n to its neighbour. In the case of the square lattice shown in Fig.1 they are:

$$\begin{aligned}
&n_1 = \vec{i}, n_2 = -\vec{i}\ n_3 = \vec{j}, n_4 = -\vec{j}\\
&n_5 = \frac{1}{\sqrt{2})}(\vec{i}+\vec{j}), n_6 = \frac{1}{\sqrt{2}}(-\vec{i}+\vec{j})\\
&n_7 = \frac{1}{\sqrt{2}}(\vec{i}-\vec{j}), n_8 = \frac{1}{\sqrt{2}}(-\vec{i}-\vec{j})
\end{aligned} \tag{2}$$

The operations like $(D_1-1),(D_1-1)^2, etc$ act as operators, not as multipliers, e.g.,

$$((D_1-1)\vec{U}_{m,n}\cdot\vec{n}_1)^3 = ((D_1-1)u_{m,n})^3 = (D_1u_{m,n}-u_{m,n})^3 = (u_{m+1,n}-u_{m,n})^3 \neq (D_1-1)^3u_{m,n}^3.$$

Some other operators are presented in the Appendix.

3. Nonlinear equations of motion

In order to obtain discrete equations of motion, it is necessary to determine the form of the elastic energy. It is known from Hooke's law that the forces acting between particles are expressed via the product of the springs elongations and corresponding linear spring rigidities C_1, C_2. The nonlinearity is introduced in the interparticle forces by taking into account terms with quadratic dependency on elongations multiplied by the coefficients Q_1 or Q_2. Finally, two-dimensional modelling is achieved by acting with shift operators on $\vec{U}_{m,n} \cdot \vec{n}_j$, where $\vec{n}_j$ are defined by Eqs. (2).

Then the potential energy for the particle *m,n* interacting with eight neighbours may be written as:

$$\begin{aligned} V_{m,n} = {} & \frac{C_1}{2}(((D_1-1)\vec{U}_{m,n}\cdot\vec{n}_1)^2 + ((D_1^\dagger-1)\vec{U}_{m,n}\cdot\vec{n}_2)^2 + ((D_2-1)\vec{U}_{m,n}\cdot\vec{n}_3)^2 \\ & + ((D_2^\dagger-1)\vec{U}_{m,n}\cdot\vec{n}_4)^2) + \frac{C_2}{2}(((D_1D_2-1)\vec{U}_{m,n}\cdot\vec{n}_5)^2 + ((D_1^\dagger D_2^\dagger-1)\vec{U}_{m,n}\cdot\vec{n}_6)^2 + \\ & ((D_1^\dagger D_2-1)\vec{U}_{m,n}\cdot\vec{n}_7)^2 + ((D_1D_2^\dagger-1)\vec{U}_{m,n}\cdot\vec{n}_8)^2) + \frac{Q_1}{3}(((D_1-1)\vec{U}_{m,n}\cdot\vec{n}_1)^3 + \\ & ((D_1^\dagger-1)\vec{U}_{m,n}\cdot\vec{n}_2)^3 + ((D_2-1)\vec{U}_{m,n}\cdot\vec{n}_3)^3 + ((D_2^\dagger-1)\vec{U}_{m,n}\cdot\vec{n}_4)^3) \\ & + \frac{Q_2}{3}(((D_1D_2-1)\vec{U}_{m,n}\cdot\vec{n}_5)^3 + ((D_1^\dagger D_2^\dagger-1)\vec{U}_{m,n}\cdot\vec{n}_6)^3 + \\ & ((D_1^\dagger D_2-1)\vec{U}_{m,n}\cdot\vec{n}_7)^3 + ((D_1D_2^\dagger-1)\vec{U}_{m,n}\cdot\vec{n}_8)^3) \end{aligned} \tag{3}$$

The equations of motion are obtained using the Hamilton - Ostrogradsky variational principle for which the Lagrangian is needed in the form:

$$L_{m,n} = T_{m,n} - V_{m,n} = \frac{m}{2}(\dot{u}_{m,n}^2 + \dot{v}_{m,n}^2) - V_{m,n}, \tag{4}$$

The discrete equations of motion are:

$$\begin{aligned} m\ddot{u}_{m,n} = {} & C_1(D_1 + D_1^\dagger - 2)u_{m,n} + C_2(D_1D_2 + D_1^\dagger D_2 + D_1D_2^\dagger + D_1^\dagger D_2^\dagger - 4)u_{m,n} + \\ & + C_2(D_1D_2 + D_1^\dagger D_2 + D_1D_2^\dagger + D_1^\dagger D_2^\dagger)v_{m,n} + Q_1((D_1u_{m,n} - u_{m,n})^2 + (D_1^\dagger u_{m,n} - u_{m,n})^2) + \\ & + Q_2((D_1D_2u_{m,n} - u_{m,n} + D_1D_2v_{m,n} - v_{m,n})^2 + (u_{m,n} - D_1^\dagger D_2^\dagger u_{m,n} + v_{m,n} - D_1^\dagger D_2^\dagger v_{m,n})^2 \\ & - (u_{m,n} - D_1^\dagger D_2 u_{m,n} + D_1^\dagger D_2 v_{m,n} - v_{m,n})^2 + (D_1D_2^\dagger u_{m,n} - u_{m,n} + v_{m,n} - D_1D_2^\dagger v_{m,n})^2) \end{aligned} \tag{5}$$

$$\begin{aligned} m\ddot{v}_{m,n} = {} & C_1(D_2 + D_2^\dagger - 2)v_{m,n} + C_2(D_1D_2 + D_1^\dagger D_2 + D_1D_2^\dagger + D_1^\dagger D_2^\dagger - 4)v_{m,n} + \\ & + C_2(D_1D_2 + D_1^\dagger D_2 + D_1D_2^\dagger + D_1^\dagger D_2^\dagger)u_{m,n} + Q_1((D_1u_{m,n} - u_{m,n})^2 + (D_1^\dagger u_{m,n} - u_{m,n})^2) + \\ & + Q_2((D_1D_2u_{m,n} - u_{m,n} + D_1D_2v_{m,n} - v_{m,n})^2 - (u_{m,n} - D_1^\dagger D_2^\dagger u_{m,n} + v_{m,n} - D_1^\dagger D_2^\dagger v_{m,n})^2 \\ & + (u_{m,n} - D_1^\dagger D_2 u_{m,n} + D_1^\dagger D_2 v_{m,n} - v_{m,n})^2 - (D_1D_2^\dagger u_{m,n} - u_{m,n} + v_{m,n} - D_1D_2^\dagger v_{m,n})^2) \end{aligned} \tag{6}$$

The linearized equations may be solved giving rise to the dispersion relation. In the nonlinear case, analytical solution of the discrete equations is unknown.

Let us consider long waves propagation. In this case, a continuum limit of Eqs. (5), (6) may be obtained by correspondence of the continuum functions *u(x,y,t)*, *v(x,y,t)* to the discrete functions respectively. The continuum analogues of the discrete functions $u_{m+i,n+j}$, $v_{m+i,n+j}$ are obtained using the Taylor series expansions of the functions *u(x,y,t)*, *v(x,y,t)* raised to the power of *h* using the exponent expansions of the shift operators given in the previous section.

The nonlinear problem is rather complicated in the general case. That is why we consider plane waves propagation as a first step of nonlinear waves study. This is a typical simplification in nonlinear lattice problems [24]. Assume no variations in the vertical direction (along the y axis) and no vertical displacements, ($v_{m,n} = 0$) to take place. This corresponds to the plane waves propagation when the function *u(x,t)* does not depend on *y*. Then only continuum limit of Eq. (5) retains, while Eq. (6) is satisfied identically. Even in this case the nonlinear continuum part remains complicated. However, when weakly nonlinear case is studied, only leading nonlinear terms may be retained, here in the form of quadratic nonlinear term

$$m\ddot{u} = h^2(C_1 + C_2)u_{xx} + 2h(Q_1 + 2Q_2)u_x u_{xx} + \frac{h^4}{12}(C_1 + C_2)u_{xxxx} \tag{7}$$

Equation (7) may be rewritten for the strain function $v = u_x$,

$$m\ddot{v} = h^2(C_1 + C_2)v_{xx} + h(Q_1 + 2Q_2)(v^2)_{xx} + \frac{h^4}{12}(C_1 + C_2)v_{xxxx}, \tag{8}$$

in the familiar form of the Boussinesq equation. This is integrable equation [23], in particular, it admits localized traveling wave solution keeping its shape and velocity on propagation. The signs of nonlinear rigidities Q_1 and Q_2 affect the type of the wave: negative sign of $Q_1 + 2Q_2$ results in the compression localized wave while the positive sign gives rise to the tensile wave.

4. Conclusion

The main finding of the paper concerns in generalization of the model based on the shift operator [1] on the two-dimensional nonlinear case. It is shown, that the nonlinear contribution in the energy may be modeled using the shift operators, and introduction of the normal vectors allows us to develop a two-dimensional modeling. The plane nonlinear longitudinal waves were considered only as a first step to see how the shift operator formalism works. An anticipated advantage of the formalism is in the development of nonlocal models that was demonstrated in the linear one-dimensional case in [1]. Hence, the further investigation is aimed at the development of nonlocal and nonlinear two-dimensional models.

The continuum equation (8) is obtained in the long-wave limit. Derivation of the short wavelength equations may be done similar to that shown in Refs. [24-26].

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Appendix

Shift Operations. Here the operations concerning the shift operators are illustrated for the multiplicative operations for the easier grasp on the method's application. For the sake of the example the C_3 coefficient for diagonal interactions is introduced. Operator multiplication always implies taking into consideration both vertical and horizontal directions, so, after multiplying $U_{m,n}$ on n_i there always will be both $u_{m,n}$ and $v_{m,n}$ left:

$$C_3 D_1 D_2(\mathbf{U}_{m,n} \cdot \mathbf{n_5}) = C_3 D_1 D_2(u_{m,n}\mathbf{i} + v_{m,n}\mathbf{j}) \cdot \frac{1}{\sqrt{2}}(\mathbf{i}+\mathbf{j}) = \frac{C_3}{\sqrt{2}} D_1 D_2(u_{m,n} + v_{m,n}) =$$

$$\frac{C_3}{\sqrt{2}}(u_{m+1,n+1} + v_{m+1,n+1})$$

More complex example consists in applying this operator in the expression such as follows:

$$C_3((D_1 D_2 - 1)\vec{U}_{m,n} \cdot \vec{n_5})^2 = C_3((D_1 D_2 \vec{U}_{m,n} - \vec{U}_{m,n}) \cdot \frac{1}{\sqrt{2}}(\vec{i} + \vec{j}))^2 =$$

$$\frac{C_3}{2}(D_1 D_2(u_{m,n} + v_{m,n}) - u_{m,n} - v_{m,n})^2 = \frac{C_3}{2}(u_{m+1,n+1} - u_{m,n} + v_{m+1,n+1} - v_{m,n})^2$$

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