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General lattice model of gradient elasticity

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In this paper, new lattice model for the gradient elasticity is suggested. This lattice model gives a microstructural basis for second-order strain-gradient elasticity of continuum that is described by the linear elastic constitutive relation with the negative sign in front of the gradient. Moreover, the suggested lattice model allows us to have a unified description of gradient models with positive and negative signs of the strain gradient terms. Possible generalizations of this model for the high-order gradient elasticity and three-dimensional case are also suggested.

Keywords: Lattice model; gradient elasticity; long-range interaction; non-local continuum.

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1. Introduction

The two most widely used theories of elastic deformation in solid materials are a microscopic approach based on the statistical mechanics of lattices[1–3] and the quantum theory of solid-states,[4] and a macroscopic approach based on the classical continuum mechanics.[5,6] Continuum elasticity is a phenomenological theory representing continuum limit of lattice dynamics, where the length-scales are much larger than inter-atomic distances. Nonlocal elasticity theory is based on the assumption that the forces between material points can be at long-range in character, thus reflecting the long-range character of interatomic and intermolecular forces. In general, the nonlocal continuum models describe materials whose behavior at any point depends on the states of all other points in the media, in addition to its own state and the state of external fields. Such considerations are well-known in solid-state physics, where the nonlocal interactions between the atoms and molecules are prevalent in determining the properties of the media and materials.

The theory of nonlocal continuum mechanics was formally initiated by Refs. 7–9. Kroner[7] indicated the relation between nonlocal elasticity theory of materials with long range cohesive forces. Eringen and Edelen[9] provided derivation of the constitutive equations for the nonlocal elasticity. Eringen and Kim[10] described a relation between nonlocal elasticity and lattice dynamics. Kunin described the physical aspects of nonlocal elasticity in Ref. 11, and studied various problems in Fourier space. In Ref. 12, Eringen considered a unified approach to field theories for elastic solids, viscous fluids, and heat-conducting electromagnetic solids and fluids that include nonlocal effects. Rogula[13] considered the mathematical aspects of nonlocal elasticity models, proposed different types of nonlocal constitutive relations between stress and strain, and applied it to various problems in continuum mechanics. Nonlocal continuum mechanics has been treated with two different approaches:[13,14] the gradient elasticity theory (weak nonlocality) and the integral nonlocal theory (strong nonlocality). In this paper, we discuss the gradient models of nonlocality elasticity. Usually two classes of gradient models are distinguished by the different signs of the strain gradient terms in the constitutive relations for the strain ε_{ij} and the stress σ_{ij}:

$$\sigma_{ij} = (\lambda \varepsilon_{kk} \delta_{ij} + 2\mu \varepsilon_{ij}) \pm l^2 \Delta (\lambda \varepsilon_{kk} \delta_{ij} + 2\mu \varepsilon_{ij}) \,, \tag{1}$$

where λ and μ are the Lame coefficients, l is the scale parameter. If $l^2 = 0$, we have the classical case of the linear elastic constitutive relations for isotropic case that is the well-known Hooke's law.

The first class of gradient elasticity models are described by Eq. (1) with the positive sign in front of gradient. The main motivation to use this form of the gradient elasticity is the description of dispersive wave propagation through heterogeneous media. In many studies, gradient elasticity models with the positive sign in (1) have been derived from associated lattice models by the continualization procedure for the response of a lattice.[16–18]

The second class of gradient elasticity models are described by Eq. (1) with the negative sign in front of the gradient. The strain gradients in Eq. (1) with the negative sign are equivalent to those derived from the positive-definite deformation energy density, and therefore these models of the strain gradients are stable.

The positive sign of the strain gradient term in Eq. (1) makes this term destabilizing. The corresponding equation for the displacements is unstable for wave numbers[15,17,19,20] $k > 1/l^2$. In dynamics the instabilities lead to an unbounded growth of the response in time without external work. It is known the instabilities are related to loss of uniqueness in static boundary value problems. Instabilities in statics and dynamics for the second-gradient models with the positive sign are discussed in Ref. 21.

At this moment there is the opinion that gradient elasticity models with the negative sign in Eq. (1) cannot be obtained from lattice models.[14] It is usually assumed that this class of the second-gradient models does not have a direct relationship with discrete microstructure and lattice models.[15] It was proved that the homogenization (continualization) procedure, which is considered in Refs. 16–19 and 22, uniquely leads to a second-order strain gradient term that is preceded by a positive sign. The second-gradient model with negative sign cannot be derived by this homogenization procedure. From a mathematical point of view it is caused by properties of the Taylor series that is used in this procedure.

In this paper, we propose lattice models, that allow us to derive linear elastic constitutive relations with negative and positive signs. Moreover, the suggested lattice models give unified description of the gradient models with positive and negative signs of the strain gradient terms. To obtain continuum equation from the lattice equations, we use an approach that is suggested in Refs. 24–27.

2. Equations of Lattice Model

Let us consider the vibration of an unbounded homogeneous lattice, such that all particles are displaced from its equilibrium position in one direction, and the displacement of particle is described by a scalar field. We consider one-dimensional lattice system of interacting particles, where the equation of motion of nth particle is

$$M \frac{d^2 u_n(t)}{dt^2} = g_2 \sum_{\substack{m=-\infty \\ m \neq n}}^{+\infty} K_2(n,m) u_m(t) + g_4 \sum_{\substack{m=-\infty \\ m \neq n}}^{+\infty} K_4(n,m) u_m(t) + F(u_n(t)) \,, \quad (2)$$

where $u_n(t)$ are displacements from the equilibrium, g_2 and g_4 are coupling constants, $F(u_n)$ is the external on-site force, $K_2(n,m)$ and $K_4(n,m)$ are the functions with different power-law asymptotic behavior of the functions

$$\hat{K}_s(k) = 2 \sum_{n=1}^{\infty} K_s(n,0) \cos(kn), \quad (s = 2; 4) \quad (3)$$

for $k \to 0$. We will consider interactions terms for which the difference $\hat{K}_s(k) - \hat{K}_s(0)$ are asymptotically equivalent to $|k|^s$ as $|k| \to 0$. Note some general properties of $K_s(n,m)$, with $s = 2; 4$. The conservation law of the total momentum in lattice (2), in case of absence of external forces $F(u_n) = 0$ gives

$$\sum_{\substack{m=-\infty \\ m \neq n}}^{+\infty} K_2(n,m) = 0, \qquad \sum_{\substack{m=-\infty \\ m \neq n}}^{+\infty} K_4(n,m) = 0 \,, \quad (4)$$

for all n. For the homogeneous unbounded lattice, we have

$$K_2(n,m) = K_2(n-m), \quad K_4(n,m) = K_4(n-m) \,,$$

where elements of $K_s(n,m)$ are constrained by condition (4), and

$$\sum_m K_s(n-m) = \sum_n K_s(n-m) = 0 \,. \quad (5)$$

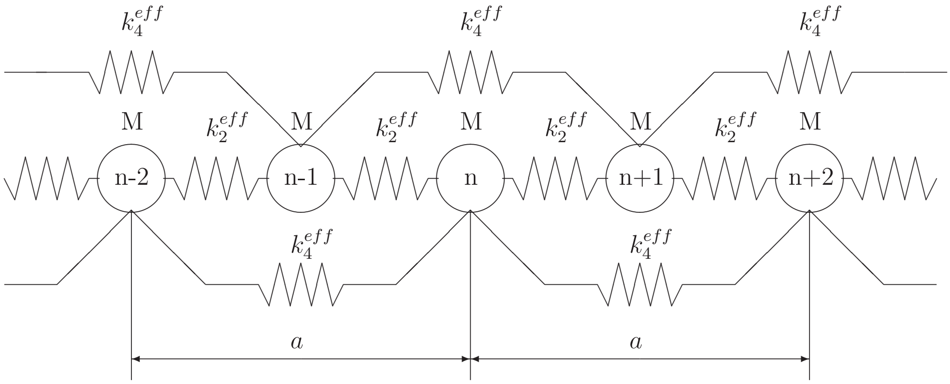

Fig. 1. Discrete mass–spring system with effective stiffness coefficients $k_2^{\text{eff}} = k_2^{\text{eff}}(g_2, g_4)$ and $k_4^{\text{eff}} = k_4^{\text{eff}}(g_2, g_4)$, the mass M and the distance a that correspond to the lattice model with coupling constants g_2 and g_4.

For a simple case, each particle is an inversion center and $K_s(n-m) = K_s(|n-m|)$, where $s = 2; 4$. Using condition (4), we can rewrite Eq. (2) as

$$M \frac{d^2 u_n}{dt^2} = g_2 \sum_{\substack{m=-\infty \\ m \neq n}}^{+\infty} K_2(|n-m|)(u_n - u_m) + g_4 \sum_{\substack{m=-\infty \\ m \neq n}}^{+\infty} K_4(|n-m|)(u_n - u_m) + F(u_n) . \tag{6}$$

In this form of equation of motion, the interaction terms are translation invariant. It should be noted that the noninvariant terms lead to divergences in the continuum models.[27]

Let us give an effective discrete mass–spring system for the suggested lattice model (6). In Fig. 1, we present the nearest-neighbor and next-nearest-neighbor interactions only. In general, functions $K_2(|n-m|)$ and $K_4(|n-m|)$ describe long-range interactions with the power-law asymptotic (3).

3. From Lattice Model to Continuum Model

Let us consider a set of operations[24,25,27] that transforms the equations of motion of the lattice model into a continuum equation for the displacement field $u(x,t)$. We assume that $u_n(t)$ are Fourier coefficients of the field $\hat{u}(k,t)$ on $[-K_0/2, K_0/2]$ that is described by the equations:

$$\hat{u}(k,t) = \sum_{n=-\infty}^{+\infty} u_n(t) e^{-ikx_n} = \mathcal{F}_\Delta\{u_n(t)\} , \tag{7}$$

$$u_n(t) = \frac{1}{K_0} \int_{-K_0/2}^{+K_0/2} dk \hat{u}(k,t) e^{ikx_n} = \mathcal{F}_\Delta^{-1}\{\hat{u}(k,t)\} , \tag{8}$$

where $x_n = na$ and $a = 2\pi/K_0$ are distance between equilibrium positions of the lattice particles. Equations (7) and (8) are the basis for the Fourier transform $\mathcal{F}_\Delta$

and the inverse Fourier series transform $\mathcal{F}_{\Delta}^{-1}$. The Fourier transform can be derived from (7) and (8) in the limit as $a \to 0$ ($K_0 \to \infty$). In this limit ($a \to 0$ or $K_0 \to \infty$), the sum becomes the integral, and Eqs. (7) and (8) become

$$\tilde{u}(k,t) = \int_{-\infty}^{+\infty} dx e^{-ikx} u(x,t) = \mathcal{F}\{u(x,t)\}\,, \tag{9}$$

$$u(x,t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk e^{ikx} \tilde{u}(k,t) = \mathcal{F}^{-1}\{\tilde{u}(k,t)\}\,. \tag{10}$$

Here we use the lattice function

$$u_n(t) = \frac{2\pi}{K_0} u(x_n, t)$$

with continuous $u(x,t)$, where

$$x_n = na = \frac{2\pi n}{K_0} \to x\,.$$

We assume that $\tilde{u}(k,t) = \mathcal{L}\hat{u}(k,t)$, where $\mathcal{L}$ denotes the passage to the limit $a \to 0$ ($K_0 \to \infty$), i.e. the function $\tilde{u}(k,t)$ can be derived from $\hat{u}(k,t)$ in the limit $a \to 0$. Note that $\tilde{u}(k,t)$ is a Fourier transform of the field $u(x,t)$. The function $\hat{u}(k,t)$ is a Fourier series transform of $u_n(t)$, where we can use $u_n(t) = (2\pi/K_0)u(na,t)$.

We can state that a lattice model transforms into a continuum model by the combination $\mathcal{F}^{-1}\mathcal{L}\mathcal{F}_{\Delta}$ of the following operation. The Fourier series transform:

$$\mathcal{F}_{\Delta} : \, u_n(t) \to \mathcal{F}_{\Delta}\{u_n(t)\} = \hat{u}(k,t)\,. \tag{11}$$

The passage to the limit $a \to 0$:

$$\mathcal{L} : \, \hat{u}(k,t) \to \mathcal{L}\{\hat{u}(k,t)\} = \tilde{u}(k,t)\,. \tag{12}$$

The inverse Fourier transform:

$$\mathcal{F}^{-1} : \, \tilde{u}(k,t) \to \mathcal{F}^{-1}\{\tilde{u}(k,t)\} = u(x,t)\,. \tag{13}$$

These operations allow us to get a continuum model from the lattice model.[24,25,27]

4. Lattice Model with Nearest-Neighbor Interaction

Let us derive the usual elastic equation from the lattice model with the nearest-neighbor interaction with coupling constant $g_2 = K$ by the method suggested in Refs. 24, 25 and 27. We will use Eq. (2) with

$$\sum_{\substack{m=-\infty \\ m \neq n}}^{+\infty} K_2(n,m) u_m(t) = u_{n+1}(t) - 2u_n(t) + u_{n-1}(t), \quad K_4(n,m) = 0\,, \tag{14}$$

where the term $K_2(n,m)$ describes the nearest-neighbor interaction.

We can give the following statement regarding the lattice model with the nearest-neighbor interaction and the corresponding continuum equation that is obtained in the limit $a \to 0$.

Proposition 1. *In the continuous limit* $(a \to 0)$, *the lattice equations of motion*

$$M \frac{d^2 u_n(t)}{dt^2} = K \cdot (u_{n+1}(t) - 2u_n(t) + u_{n-1}(t)) + F(u_n(t)) \tag{15}$$

are transformed by the combination $\mathcal{F}^{-1}\mathcal{L}\mathcal{F}_{\Delta}$ *of the operations* (11)–(13) *into the continuum equation:*

$$\frac{\partial^2 u(x,t)}{\partial t^2} = C_e^2 \frac{\partial^2 u(x,t)}{\partial x^2} + \frac{1}{\rho} f(u) \,, \tag{16}$$

where $C_e^2 = E/\rho = Ka^2/M$ *is a finite parameter and* $f(u) = F(u)/(Aa)$.

Proof. To derive the equation for the field $\hat{u}(k,t)$, we multiply Eq. (15) by $\exp(-ikna)$, and summing over n from $-\infty$ to $+\infty$. Then

$$M \sum_{n=-\infty}^{+\infty} e^{-ikna} \frac{d^2 u_n}{dt^2} = K \cdot \sum_{n=-\infty}^{+\infty} e^{-ikna} (u_{n+1} - 2u_n + u_{n-1}) + \sum_{n=-\infty}^{+\infty} e^{-ikna} F(u_n) \,. \tag{17}$$

The first term on the right-hand side of (17) is

$$\begin{aligned} K \cdot \sum_{n=-\infty}^{+\infty} e^{-ikna} K_2(n,m) u_n &= K \cdot \sum_{n=-\infty}^{+\infty} e^{-ikna} (u_{n+1} - 2u_n + u_{n-1}) \\ &= K \cdot \sum_{n=-\infty}^{+\infty} e^{-iknd} u_{n+1} - 2K \cdot \sum_{n=-\infty}^{+\infty} e^{-iknd} u_n \\ &\quad + K \cdot \sum_{n=-\infty}^{+\infty} e^{-ikna} u_{n-1} \\ &= e^{ika} K \cdot \sum_{m=-\infty}^{+\infty} e^{-ikma} u_m - 2K \cdot \sum_{n=-\infty}^{+\infty} e^{-ikna} u_n \\ &\quad + e^{-ikd} K \cdot \sum_{j=-\infty}^{+\infty} e^{-ikja} u_j \,. \end{aligned}$$

Using the definition of $\hat{u}(k,t)$, we obtain

$$\begin{aligned} K \cdot \sum_{n=-\infty}^{+\infty} e^{-ikna} K_2(n,m) u_n &= K \cdot (e^{ikd} \hat{u}(k,t) - 2\hat{u}(k,t) + e^{-ika} \hat{u}(k,t)) \\ &= K \cdot (e^{ika} + e^{-ika} - 2) \hat{u}(k,t) \\ &= 2K \cdot (\cos(ka) - 1) \hat{u}(k,t) \\ &= -4K \cdot \sin^2 \left(\frac{ka}{2} \right) \hat{u}(k,t) \,. \end{aligned} \tag{18}$$

Substitution of (18) into (17) gives

$$M\frac{\partial^2 \hat{u}(k,t)}{\partial t^2} = -4K \cdot \sin^2\left(\frac{ka}{2}\right) \hat{u}(k,t) + \mathcal{F}_{\Delta}\{F(u_n(t))\}. \tag{19}$$

For $a \to 0$, the asymptotic behavior of the sine is $\sin(ka/2) = ka/2 + O((ka)^3)$, then

$$-4\sin^2\left(\frac{ka}{2}\right) = -(ka)^2 + O((ka)^4).$$

Using the finite parameter $C_e^2 = Ka^2/M$, the transition to the limit $a \to 0$ in Eq. (19) gives

$$\frac{\partial^2 \tilde{u}(k,t)}{\partial t^2} = -C_e^2 k^2 \tilde{u}(k,t) + \frac{1}{M}\mathcal{F}\{F(u)\}\,, \tag{20}$$

where

$$\rho = \frac{M}{Aa}, \quad E = \frac{Ka}{A}, \quad C_e^2 = \frac{E}{\rho} = \frac{Ka^2}{M}\,. \tag{21}$$

The inverse Fourier transform $\mathcal{F}^{-1}$ of (20) has the form

$$\frac{\partial^2 \mathcal{F}^{-1}\{\tilde{u}(k,t)\}}{\partial t^2} = -C_e^2 \mathcal{F}^{-1}\{k^2 \tilde{u}(k,t)\} + \frac{1}{\rho} f(u),$$

where $f(u) = F(u)/(Aa)$ is the force density. Then we can use $\mathcal{F}^{-1}\{\tilde{u}(k,t)\} = \tilde{u}(x,t)$, and the connection between derivatives and its Fourier transform: $\mathcal{F}^{-1}\{k^2\tilde{u}(k,t)\} = \partial^2 u(x,t)/\partial x^2$. As a result, we obtain the continuum equation (16). This ends the proof. □

As a result, we prove that the lattice equations (15) in the limit $a \to 0$ give the continuum equation with derivatives of second order only. This conclusion agrees with the results of Ref. 23, where the relation

$$\exp i\left(-ia\frac{\partial}{\partial x}\right) u(x,t) = u(x+a,t)$$

and the representation of (15) by pseudo-differential equation are used.

5. From General Lattice Model to Gradient Elasticity Model

Let us consider the lattice model that is described by (2), where the terms $K_s(n,m)$ with $s = 2$ and $s = 4$ satisfy the conditions

$$K_s(n,m) = K_s(|n-m|), \quad \sum_{n=1}^{\infty} |K_s(n)|^2 < \infty\,. \tag{22}$$

To describe gradient elasticity models, we consider the inter-particle interactions, that are described by $K_s(n)$ ($s = 2$ or $s = 4$) of the following special type. We assume that the function

$$\hat{K}_s(k) = \sum_{\substack{n=-\infty \\ n\neq 0}}^{+\infty} e^{-ikn} K_s(n) = 2\sum_{n=1}^{\infty} K_s(n)\cos(kn)\,, \tag{23}$$

satisfies the condition

$$\lim_{k\to 0} \frac{\hat{K}_s(k) - \hat{K}_s(0)}{|k|^s} = A_s\,, \tag{24}$$

where $0 < |A_s| < \infty$. Condition (24) means that

$$\hat{K}_s(k) - \hat{K}_s(0) = A_s|k|^s + R_s(k)\,, \tag{25}$$

for $k \to 0$, where $\lim_{k\to 0} R_s(k)/|k|^s = 0$. This also means that we can consider arbitrary functions $K_s(|n-m|)$ for which $\hat{K}_s(k) - \hat{K}_s(0)$ are asymptotically equivalent to $|k|^s$ as $|k| \to 0$.

As an example of the interaction terms $K_s(|n-m|)$, which give the continuum equations of gradient elasticity models, we consider the function

$$K_s(|n-m|) = \frac{(-1)^{|n-m|}}{2\Gamma(s/2+1+|n-m|)\Gamma(s/2+1-|n-m|)}\,. \tag{26}$$

We use 2 in the denominator to cancel with 2 from Eq. (23). The terms $K_s(|n-m|)$ are considered for $n \neq m$, i.e. $|n-m| \neq 0$. For $s = 2j$, we have $K_s(|n-m|) = 0$ for all $|n-m| \geq j+1$. The function $K_s(n-m)$ with even value of $s = 2j$ describes an interaction of the n-particle with $2j$ particles with numbers $n \pm 1, \ldots, n \pm j$. To represent properties of (26), we can consider the function

$$f_K(x,y) = \mathrm{Re}\,[K_y(x)] = \frac{\mathrm{Re}\,[(-1)^{|x|}]}{2\Gamma(y/2+1+|x|)\Gamma(y/2+1-|x|)} \tag{27}$$

of two continuous variables x and $y > 0$. Note that $\mathrm{Re}\,[(-1)^{|x|}] = (-1)^{|x|}$ for integer $x = n - m$. The plots of the function (27) are presented by Figs. 2 and 3 for different ranges of x and y. This function decays rapidly with growth x and y. The function (27) defines the interaction terms $K_s(|n-m|)$ by the equation $K_s(|n-m|) = f_K(|n-m|, s)$.

Using an inverse relation to (23) with $\hat{K}_s(k) = |k|^s$ that has the form

$$K_s(n) = \frac{1}{\pi}\int_0^{\pi} k^s \cos(nk)dk\,,$$

we get another example of $K_s(|n-m|)$ in the form

$$K_s(|n-m|) = \frac{\pi^s}{s+1}\,{}_1F_2\left(\frac{s+1}{2}; \frac{1}{2}, \frac{s+3}{2}; -\frac{\pi^2(n-m)^2}{4}\right)\,, \tag{28}$$

where ${}_1F_2$ is the Gauss hypergeometric function (see Chapter II in Ref. 40). Note that the interactions with (28) for $s = 2$ and $s = 4$ are long-range interactions of n-particle with all other particles ($m \in \mathbb{N}$). It is easy to see that expression (28) is more complicated than (26).

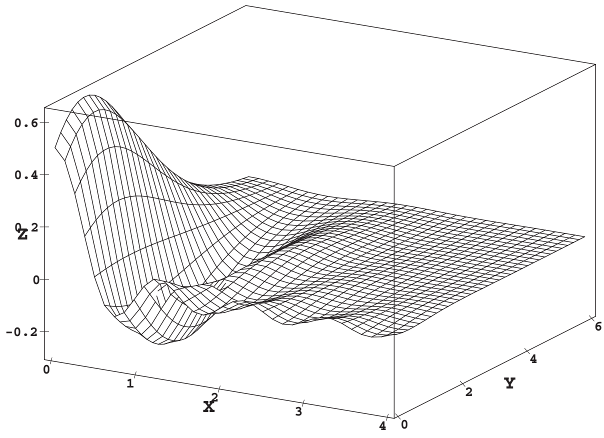

Fig. 2. Plot of the function (27) for the range $x \in [0, 4]$ and $y \in [0, 6]$.

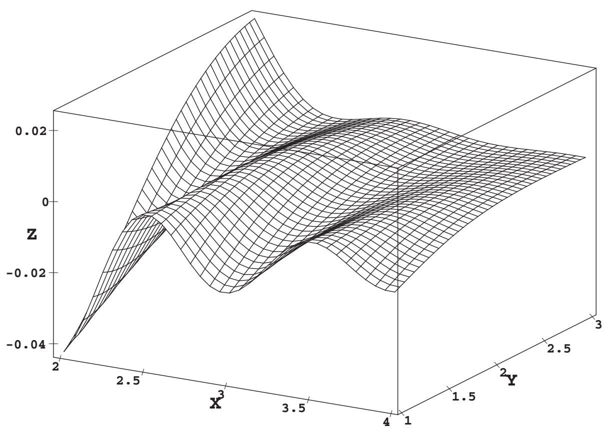

Fig. 3. Plot of the function (27) for the range $x \in [2, 4]$ and $y \in [1, 3]$.

For $s = 2$, we can also use the long-range interactions in the following two forms

$$K_2(|n-m|) = \frac{(-1)^{|n-m|}}{(n-m)^2}, \quad K_2(|n-m|) = \frac{1}{|n-m|^{\alpha}}, \quad (\alpha \geq 3). \tag{29}$$

A main advantage of the interaction in the forms (26) and (28) is a possibility to use for other generalizations for the case of the high-order gradient elasticity by using arbitrary integer values of s and the fractional generalization of gradient elasticity by non-integer values of s.

Proposition 2. *The lattice equations*

$$M\frac{d^2u_n}{dt^2} = g_2 \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} K_2(|n-m|)[u_n-u_m] + g_4 \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} K_4(|n-m|)[u_n-u_m] + F(u_n)\,, \tag{30}$$

where g_2 and g_4 are coupling constants, $K_2(|n-m|)$ and $K_4(|n-m|)$ are defined by (26), *$u_n = u_n(t)$, are transformed by the combination $\mathcal{F}^{-1}\mathcal{L}\mathcal{F}_\Delta$ of the operations* (11)–(13) *into the continuum equation:*

$$\frac{\partial^2 u(x,t)}{\partial t^2} - G_2\frac{\partial^2 u(x,t)}{\partial x^2} + G_4\frac{\partial^4 u(x,t)}{\partial x^4} - \frac{1}{\rho}f(u(x,t)) = 0\,, \tag{31}$$

where

$$G_2 = \frac{g_2 a^2}{4M}, \quad G_4 = \frac{g_4 a^4}{48M} \tag{32}$$

are finite parameters, $\rho = M/(Aa)$ is the mass density and $f(u) = F(u)/(Aa)$ is the force density.

Proof. To derive the equation for the field $\hat{u}(k,t)$, we multiply Eq. (30) by $\exp(-ikna)$, and summing over n from $-\infty$ to $+\infty$. Then

$$M\sum_{n=-\infty}^{+\infty} e^{-ikna}\frac{d^2}{dt^2}u_n(t) = \sum_{n=-\infty}^{+\infty}\sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty}\sum_{s=2;4} e^{-ikna} g_s K_s(|n-m|)[u_n-u_m]$$
$$+ \sum_{n=-\infty}^{+\infty} e^{-ikna}F(u_n)\,. \tag{33}$$

The left-hand side of (33) gives

$$\sum_{n=-\infty}^{+\infty} e^{-ikna}\frac{\partial^2 u_n(t)}{\partial t^2} = \frac{\partial^2}{\partial t^2}\sum_{n=-\infty}^{+\infty} e^{-ikna}u_n(t) = \frac{\partial^2 \hat{u}(k,t)}{\partial t^2}\,, \tag{34}$$

where $\hat{u}(k,t)$ is defined by (7). The second term of the right-hand side of Eq. (33) is $\sum_{n=-\infty}^{+\infty} e^{-ikna}F(u_n) = \mathcal{F}_\Delta\{F(u_n)\}$. The first term on the right-hand side of (33) is

$$\sum_{n=-\infty}^{+\infty}\sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikna}K_s(|n-m|)[u_n-u_m] = \sum_{n=-\infty}^{+\infty}\sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikna}K_s(|n-m|)u_n$$
$$- \sum_{n=-\infty}^{+\infty}\sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikna}K_s(|n-m|)u_m\,. \tag{35}$$

Using (7) and (22), the first term on the right-hand side of (35) gives

$$\sum_{n=-\infty}^{+\infty} \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikna} K_s(|n-m|) u_n = \sum_{n=-\infty}^{+\infty} e^{-ikna} u_n \sum_{\substack{m'=-\infty \\ m'\neq 0}}^{+\infty} K_s(m') = \hat{u}(k,t)\hat{K}_s(0)\,, \tag{36}$$

where

$$\hat{K}_s(ka) = \sum_{\substack{n=-\infty \\ n\neq 0}}^{+\infty} e^{-ikna} K_s(n) = \mathcal{F}_{\Delta}\{K_s(n)\}\,. \tag{37}$$

The second term on the right-hand side of (35) gives

$$\begin{aligned} \sum_{n=-\infty}^{+\infty} \sum_{\substack{m=-\infty \\ m\neq n}}^{+\infty} e^{-ikna} K_s(|n-m|) u_m &= \sum_{\substack{n=-\infty \\ n\neq m}}^{+\infty} e^{-ikna} K_s(|n-m|) \sum_{m=-\infty}^{+\infty} u_m \\ &= \sum_{\substack{n'=-\infty \\ n'\neq 0}}^{+\infty} e^{-ikn'a} K_s(n') \sum_{m=-\infty}^{+\infty} u_m e^{-ikma} \\ &= \hat{K}_s(ka)\hat{u}(k,t)\,. \end{aligned} \tag{38}$$

As a result, Eq. (33) has the form

$$M \frac{\partial^2 \hat{u}(k,t)}{\partial t^2} = \sum_{s=2;4} (\hat{K}_s(0) - \hat{K}_s(ka))\hat{u}(k,t) + \mathcal{F}_{\Delta}\{F(u_n)\}\,, \tag{39}$$

where $\mathcal{F}_{\Delta}\{F(u_n)\}$ is an operator notation for the Fourier series transform of $F(u_n)$.

Using the series (see Sec. 5.4.8.12 in Ref. 28) of the form

$$\sum_{n=1}^{\infty} \frac{(-1)^n}{\Gamma(\nu+1+n)\Gamma(\nu+1-n)} \cos(nk) = \frac{2^{2\nu-1}}{\Gamma(2\nu+1)} \sin^{2\nu}\left(\frac{k}{2}\right) - \frac{1}{2\Gamma^2(\nu+1)}\,,$$

where $\nu > -1/2$ and $0 < k < 2\pi$, we get for the function (23) of the form (26) the equation

$$\hat{K}_s(ak) - \hat{K}_s(0) = \frac{2^{s-1}}{\Gamma(s+1)} \sin^s\left(\frac{ak}{2}\right) = \frac{1}{2\Gamma(s+1)}|ak|^s + O(k^{s+2})\,. \tag{40}$$

Here we use $\nu = s/2$ and $\sin(k/2) = k/2 + O(k^3)$. Note that 2 in the denominator of (26) cancels with 2 from Eq. (23) in front of the sum from zero to infinity. The limit $k \to 0$ gives

$$\lim_{k\to 0} \frac{\hat{K}_s(k) - \hat{K}_s(0)}{|k|^s} = \frac{1}{2\Gamma(s+1)}, \tag{41}$$

and we have $A_s = 1/(2\Gamma(s+1))$.

The Fourier series transform $\mathcal{F}_\Delta$ of (30) gives (39). We will be interested in the limit $a \to 0$. Using (40), Eq. (39) can be written as

$$\frac{\partial^2}{\partial t^2}\hat{u}(k,t) - \frac{g_2 a^2}{M}\hat{\mathcal{T}}_{2,\Delta}(k)\hat{u}(k,t) - \frac{g_4 a^4}{M}\hat{\mathcal{T}}_{4,\Delta}(k)\hat{u}(k,t) - \frac{1}{M}\mathcal{F}_\Delta\{F(u_n(t))\} = 0\,, \quad (42)$$

where

$$\hat{\mathcal{T}}_{s,\Delta}(k) = -\frac{1}{2\Gamma(s+1)}|k|^s + a^2 O(|k|^{s+2})\,. \quad (43)$$

In the limit $a \to 0$, using

$$\hat{\mathcal{T}}_s(k) = \mathcal{L}\hat{\mathcal{T}}_{s,\Delta}(k) = -\frac{1}{2\Gamma(s+1)}|k|^s \quad (s = 2; 4)\,, \quad (44)$$

we get

$$\hat{\mathcal{T}}_2(k) = \mathcal{L}\hat{\mathcal{T}}_{2,\Delta}(k) = -\frac{1}{4}|k|^2, \quad \hat{\mathcal{T}}_4(k) = \mathcal{L}\hat{\mathcal{T}}_{4,\Delta}(k) = -\frac{1}{48}|k|^4\,. \quad (45)$$

The passage to the limit $a \to 0$ for the third term of (42) gives $\mathcal{F}_\Delta F(u_n) \to \mathcal{L}\mathcal{F}_\Delta F(u_n)$. Then

$$\mathcal{L}\mathcal{F}_\Delta\{F(u_n)\} = \mathcal{F}\{\mathcal{L}F(u_n)\} = \mathcal{F}\{F(\mathcal{L}u_n)\} = \mathcal{F}\{F(u(x,t))\}\,, \quad (46)$$

where we use $\mathcal{L}\mathcal{F}_\Delta = \mathcal{F}\mathcal{L}$.

As a result, Eq. (42) in the limit $a \to 0$ gives

$$\frac{\partial^2}{\partial t^2}\tilde{u}(k,t) - G_2\hat{\mathcal{T}}_2(k)\tilde{u}(k,t) - G_4\hat{\mathcal{T}}_4(k)\tilde{u}(k,t) - \frac{1}{M}\mathcal{F}\{F(u(x,t))\} = 0\,, \quad (47)$$

where $\tilde{u}(k,t) = \mathcal{L}\hat{u}(k,t)$, and we use finite parameters G_2 and G_4, that are defined by (32).

The inverse Fourier transform of (47) is

$$\frac{\partial^2}{\partial t^2}u(x,t) - G_2\mathcal{T}_2(x)u(x,t) - G_4\mathcal{T}_4(x)u(x,t) - \frac{1}{\rho}f(u(x,t)) = 0\,, \quad (48)$$

where the finite parameters G_2 and G_4 are defined by (32). Using (48) the operators $\mathcal{T}_2(x)$ and $\mathcal{T}_4(x)$ are defined by

$$\mathcal{T}_2(x) = \mathcal{F}^{-1}\{\hat{\mathcal{T}}_2(k)\} = +\frac{\partial^2}{\partial x^2}, \quad \mathcal{T}_4(x) = \mathcal{F}^{-1}\{\hat{\mathcal{T}}_4(k)\} = -\frac{\partial^4}{\partial x^4}. \quad (49)$$

Here, we have used the connection between the derivatives of the second and fourth orders and their Fourier transforms $k^2 \leftrightarrow -\partial^2/\partial x^2$ and $k^4 \leftrightarrow +\partial^4/\partial x^4$, and Eq. (45).

As a result, we obtain the continuum equation (31). This ends the proof. □

Proposition 2 illustrates the close relation between the discrete microstructure and the gradient nonlocal continuum. Let us consider special cases of the suggested model.

Lattice equations (30) have two parameters g_2 and g_4. The corresponding Eq. (31) for the elastic continuum has two finite parameters G_2 and G_4. If we use $g_2 = 4K$ and $g_4 = 0$, then $G_2 = C_e^2 = Ka^2/M$, $G_4 = 0$, and we get Eq. (16). If we assume that $g_2 = 4K$ and $g_4 = -4K$, then $G_2 = C_e^2 = Ka^2/M$, $G_4 = C_e^2 a^2/48$ and we get the equation

$$\frac{\partial^2 u(x,t)}{\partial t^2} = C_e^2 \frac{\partial^2 u(x,t)}{\partial x^2} + \frac{a^2 C_e^2}{12} \frac{\partial^4 u(x,t)}{\partial x^4} + \frac{1}{\rho} f(u), \tag{50}$$

where $C_e = \sqrt{E/\rho}$ is the elastic bar velocity. Equation (50) can also be derived by the homogenization procedure.[16–18]

In general, the coupling constants g_2 and g_4 are independent. Therefore, the coupling constant g_4 may differ from the constant $g_2 = 4K$. If the relation of stress and displacement of the form $\varepsilon(x,t) = \partial u(x,t)/\partial x$ is used, and the continuum equation (31) is expresses as

$$\rho \frac{\partial^2 u(x,t)}{\partial t^2} = \frac{\partial \sigma(x,t)}{\partial x} + f(u),$$

where $\rho = M/(Aa)$, then the constitutive relation can be represented by

$$\sigma = E \left(\frac{g_2}{4K} \varepsilon - \frac{g_4 a^2}{48K} \frac{\partial^2 \varepsilon}{\partial x^2} \right), \tag{51}$$

where we use $E = Ka/A$. Therefore, using the correspondence principle, we will assume $g_2 = 4K$. The second-gradient parameter l is defined by the relation

$$l^2 = \frac{|g_4| a^2}{48K}, \tag{52}$$

where the sign in front of the factor l^2 in the constitutive relation is determined by the sign of the coupling constant g_4. If the constant g_4 is positive then we get the second-gradient model with negative sign. As a result the second-gradient model with positive and negative signs

$$\sigma = E \left(\varepsilon - \mathrm{sgn}(g_4) l^2 \frac{\partial^2 \varepsilon}{\partial x^2} \right) \tag{53}$$

can be derived from a microstructure of lattice particles by suggested approach. The proposed model as shown above uniquely leads to second-order strain gradient terms that are preceded by the positive and negative signs. It should be noted that positive value of coupling constant g_4 of lattice model can lead to effective stiffness coefficient of the next-nearest-neighbor interaction with non-convex elastic energy potentials in the effective discrete mass–spring system. The strain gradients in continuum equation with the negative sign are equivalent to those derived from the positive-definite deformation energy density, and therefore these continuum models are stable. The lattice models with negative value of coupling constant g_4 of lattice model leads to the continuum equation with the positive sign in front of the parameter l^2. This continuum equation is unstable for wave numbers $k > 1/l^2$ The instability leads to an unbounded growth of the response in time without external work.

6. Possible Extensions of General Lattice Model

The suggested lattice model can be generalized and extended for the high-order gradient elasticity and for three-dimensional lattice models. Let us give some details about these generalizations.

We can consider a generalization of the suggested lattice model by using the sum of the functions (26) with the even value s. Using the functions (26) with $s = 6$ and other even values, we can consider the lattice models for high-order gradient elasticity.[15,22,29] We can state that the lattice equations

$$M \frac{d^2 u_n(t)}{dt^2} = \sum_{j=1}^{N} g_{2j} \sum_{\substack{m=-\infty \\ m \neq n}}^{+\infty} K_{2j}(|n-m|)(u_n(t) - u_m(t)) + F(u_n)\,, \tag{54}$$

where g_{2j} $(j = 1, \dots, N)$ are coupling constants, and $K_{2j}(|n-m|)$ are defined by (26), are transformed by the combination $\mathcal{F}^{-1}\mathcal{L}\mathcal{F}_{\Delta}$ of the operations (11)–(13) into the continuum equation

$$\frac{\partial^2 u(x,t)}{\partial t^2} + \sum_{j=1}^{N} (-1)^j G_{2j} \frac{\partial^{2j} u(x,t)}{\partial x^{2j}} - \frac{1}{\rho} f(u) = 0\,, \tag{55}$$

where $G_{2j} = g_{2j} a^{2j}/(2\Gamma(2j+1))$, $(j = 1, \dots, N)$ are finite parameters. The proof of this statement is similar to the proof of Proposition 2.

The suggested one-dimensional lattice model for second-gradient elasticity can also be generalized for the three-dimensional case. We may consider a three-dimensional lattice that is described by the equation

$$\frac{d^2 u^k_{\mathbf{n}}}{dt^2} = \sum_{\mathbf{m}:\mathbf{m}\neq\mathbf{n}} K^{kl}_2(\mathbf{n}-\mathbf{m})(u^l_{\mathbf{n}} - u^l_{\mathbf{m}}) + \sum_{\mathbf{m}:\mathbf{m}\neq\mathbf{n}} K^{kl}_4(\mathbf{n}-\mathbf{m})(u^l_{\mathbf{n}} - u^l_{\mathbf{m}}) + F^k(u_{\mathbf{n}})\,, \tag{56}$$

where $\mathbf{n} = (n_1, n_2, n_3)$, $k, l = 1, 2, 3$ and we assume a sum over repeated index $l = 1, 2, 3$. In the model (56), the coupling constants are included in the tensors $K^{kl}_s(\mathbf{n}-\mathbf{m}) = K^{kl}_s(\mathbf{m}-\mathbf{n})$ that are distinguished by different power-law asymptotic behavior. We assume that the functions $\hat{K}^{kl}_s(\mathbf{k}) - \hat{K}^{kl}_s(0)$ are asymptotically equivalent to $k_i k_j$ and $k_i k_j |\mathbf{k}|^2$ for $s = 2$ and $s = 4$ respectively, where

$$\hat{K}^{kl}_s(\mathbf{k}) = \sum_{\mathbf{n}} e^{-i\mathbf{k}\mathbf{n}} K^{kl}_s(\mathbf{n})\,.$$

To get continuum equation, we consider the field $u_{\mathbf{n}}(t)$ as Fourier coefficients of the function $\hat{u}(\mathbf{k}, t)$, where $\mathbf{k} = (k_1, k_2, k_3)$, by

$$\hat{u}^k(\mathbf{k}, t) = \sum_{\mathbf{n}} u^k_{\mathbf{n}}(t) e^{-i\mathbf{k}\mathbf{r}_{\mathbf{n}}}\,,$$

where $\mathbf{r}(\mathbf{n}) = \mathbf{r}_{\mathbf{n}} = \sum_{i=1}^{3} n_i \mathbf{a}_i$, with the translational vectors $\mathbf{a}_i$ of the lattice. In three-dimensional lattice model for second-gradient elasticity, we should consider interaction terms $K_s^{kl}(\mathbf{n}-\mathbf{m})$ that satisfy the conditions

$$\lim_{k_i,k_j\to 0}\frac{\hat{K}_2^{kl}(\mathbf{k})-\hat{K}_2^{kl}(0)}{k_ik_j}=A_{ij}^{kl}(2)\,,$$
$$\lim_{k_i,k_j,|\mathbf{k}|\to 0}\frac{\hat{K}_4^{kl}(\mathbf{k})-\hat{K}_4^{kl}(0)}{k_ik_j|\mathbf{k}|^2}=A_{ij}^{kl}(4),\quad (i,j=1,2,3)\,, \tag{57}$$

where $A_{ij}^{kl}(s)$ are the coupling constants. In the continuous limit ($|\mathbf{a}_i|\to 0$), the three-dimensional lattice (56) gives the continuum equations in the form

$$\frac{\partial^2 u^k(\mathbf{r},t)}{\partial t^2}-G_{ij}^{kl}(2)\frac{\partial^2 u^l(\mathbf{r},t)}{\partial x_i\partial x_j}+G_{ij}^{kl}(4)\frac{\partial^4 u^l(\mathbf{r},t)}{\partial x_i\partial x_j\partial x_m\partial x_m}-\frac{1}{\rho}f^k(u(\mathbf{r},t))=0\,, \tag{58}$$

where we assume a sum over repeated indices $i,j,l,m\in\{1,2,3\}$, and

$$G_{ij}^{kl}(2)=\frac{|\mathbf{a}_i||\mathbf{a}_j|}{M}A_{ij}^{kl}(2),\quad G_{ij}^{kl}(4)=\sum_{m=1}^{3}\frac{|\mathbf{a}_i||\mathbf{a}_j||\mathbf{a}_m|^2}{M}A_{ij}^{kl}(4), \tag{59}$$

where no summation over repeated indices. We can consider the case with $G_{ij}^{kl}(4)=l^2G_{ij}^{kl}(2)$, where $G_{ij}^{kl}(2)=C_{ikjl}$ can be considered as a stiffness tensor and l^2 is the scale parameter. For the isotropic case, we have $C_{ijkl}=\lambda\delta_{ij}\delta_{kl}+\mu(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})$. In general, Eq. (58) describes anisotropic gradient continuum. A more detailed description of the three-dimensional lattice model (56) will be made in the following article.

7. Conclusion

In this paper, lattice models for strain-gradient elasticity of continuum are suggested. The first advantage of the suggested lattice models is a possibility to consider these models as a microstructural basis of unified description of gradient models with positive and negative signs of the strain gradient terms. A second advantage of the proposed model is that it can be easily generalized to the case of the high-order gradient elasticity by using the other even values of s. Using (26) with positive integer $s=2j$, we have nonlocal interaction of the lattice particle that gives the derivatives of integer order $2j$ in the continuum equation. Three-dimensional lattice models and the correspondent continuum equation can also be formulated as (56) and (58). The third advantage of the proposed form of the interaction is that the lattice equations can be used not only for the integer but also for fractional values of the parameter s. Therefore, the suggested general lattice model can be extended on the fractional nonlocal case. The suggested types (26) and (28) of inter-particle interactions in the lattice can be used for non-integer s. If we consider interaction terms defined by (26) and (28) with non-integer $s=\alpha$, then we will get continuum equations with the Riesz fractional derivatives[41] of orders $s=\alpha$ by the methods suggested in Refs. 24 and 25. The lattice models with long-range interactions of the types (26) and (28) with non-integer $s=\alpha$, can serve as microscopic models for elastic continuum with power-law nonlocality. It allows us to derive fractional generalizations of gradient elasticity by using a microscopic approach.[30,31] We also assume that the suggested lattice model can be generalized to get discrete (lattice) models for dislocations in the gradient elasticity continuum,[32–39] and then it will be possible to extend them to the fractional nonlocal case. The suggested lattice models with long-range interactions, which are suggested for the gradient elasticity continuum, can be important to describe the nonlocal elasticity of materials at micro and nano scales,[42–45] where the interatomic and intermolecular interactions are prevalent in determining the properties of these materials.

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