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ORIGINAL ARTICLE

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Towards multi-scale continuum elasticity theory

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Abstract We propose a new method of constructing a series of nested quasicontinuum models, which describe linear elastic behavior of crystal lattices at successively smaller scales. The relevant scales are dictated by the interatomic interactions and are not arbitrary. The novelty of the model is in the use of a decomposition of the displacement field into the coarse part and the micro-level corrections. The coarse contribution is the conventional homogenized displacement field used in classical continuum elasticity. The micro-level corrections are sub-continuum fields representing the fine structure of the boundary layers exhibited by the discrete equilibrium configuration. The model is based on a multi-point Padé approximation in the Fourier space of the discrete Green's function. We systematically compare the new model with the conventional strain gradient model.

Keywords Lattice elasticity · Size effect · Quasicontinuum · Padé approximation · Nonlocal elasticity · Strain gradient elasticity

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1 Introduction

Continuum elasticity is known to represent the long wave limit of a discrete model for crystal lattices. The lattice may be viewed as comprised of periodically located mass points which interact through linear springs (see the classical reference [9] and the reviews in [7,8,10,27]). As homogenized theory, classical elasticity is scale free and does not contain internal cut offs. The background presence of the lattice is relevant only when the external length scale is of the order of inter atomic distance (size effect) or when the homogenized theory develops singularities. In those cases the discrete model exhibits localized boundary layers that are not captured by the continuum theory (e.g. [11]).

Due to analytical complexity of the discrete theories and the necessity of resolving explicitly all microscopic degrees of freedom, there have been repeated attempts to extend the continuum description of crystal lattices towards the scales where the classical theory shows its deficiency (see pioneering work [19,21,22,28,30,34,37] and some representative recent papers [2,6,15,16,18]). It has been long realized that in order to capture sub-continuum effects the augmented continuum theory must contain at least one microscopic internal length scale; sometimes the adjective "quasi-continuum" is used to emphasize the mixed discrete-continuum nature of the resulting theories (e.g. [13,22,31,38,39]). While it is understood that the internal length scale must be of the order of inter-atomic distance, the precise nature of this parameter remains obscure, and despite various suggestive derivations, its final value is typically attributed phenomenologically (see the references in [26]).

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The ambiguity also persists concerning the very character of the analytical extension of the continuum theory towards small scales and several archetypes of quasi-continuum theories have been discussed in the literature (see [24,32,33,36] for recent reviews). Roughly, the whole variety of continualization methods in lattice models can be divided into two main groups. The first group is focused on the approximation of the ground states (global minimizers) and is based on the method of Γ convergence and its higher order extensions (e.g. [11]). The second group assumes the existence of sufficiently smooth continuum field closely approximating (or even interpolating) the discrete one and associates with this continuum field an energy, which approximates the corresponding discrete energy (e.g. [8]). Although the status of the second group of methods is more ambiguous than of the first group, these approaches retain flexibility allowing one to potentially capture the local minima of the energy and even the energy barriers. In this paper we focus our attention only on the latter more versatile category of methods.

One possibility along these lines is to construct a fully nonlocal quasi-continuum model which provides maximally smooth, Shannon-type interpolation of the lattice field (e.g. [22]). Despite its internal consistency, this approach has not been very successful because the resulting continuum theory remains exactly as complex as the original discrete model. Another problem is that the maximally smooth interpolating model has no simple connection to classical elasticity and can not be easily transformed into a method of successive approximations. A different class of quasi-continuum models, whose origin can be traced to Van-der-Waals, can be obtained if the finite difference operators appearing in the discrete theory are formally expanded in Taylor series (e.g. [8,34]). The resulting theories are based on relatively low order partial differential equations and are more amenable to analysis than fully nonlocal models. Their domain of applicability, however, is rather limited due to the stringent requirement on the long wave character of the discrete fields that can be approximated this way. In particular, such strain-gradient theories can not be generically trusted at the scale of several atomic distances, making them quantitatively inadequate for the description of surface relaxation or for modeling of the core regions of defects. Despite these shortcoming the strain-gradient models maintain a clear link to classical elasticity and, when the corresponding problems are stable (well-posed), reproduce qualitatively correct picture of the boundary layer phenomena (e.g. [39]).

In addition to the above models with reasonably well specified asymptotic structure, various phenomenological theories with strong and weak nonlocality have also been proposed in the literature (e.g. [1,3,24, 32,33,35,36]). Such models usually have only very loose connection to the underlying discrete model and contain internal length scales that do not have a clear microscopic nature. A number of numerical approaches have also been developed in an attempt to match the smooth continuum behavior far away from defects and singularities with the progressively more detailed discrete modeling of the elastic fields in the core regions (e.g. [14,17,29,31]). Despite their unquestionable practical utility such models remain analytically impenetrable and can be viewed as purely computational. We should also mention a recent mathematical literature on the subject which is focussed on the re-evaluation and extension of the earlier continuum theories using rigorous methods of functional analysis (e.g. [10,11,16,25] and the literature sited therein).

In the present paper we build on the previous insights and propose a new class of quasi-continuum approximations allowing one to reproduce the mechanical behavior of a lattice at a succession of relevant scales. The approximations are based on a special multi-point Padé approximation of the Green's function for the discrete model. Behind the construction is the fractional decomposition of the inverse elasticity operator in the Fourier space. The model can be viewed as a set of successively more accurate approximations anchored at classical continuum elasticity which represents the coarse grained limit. When no truncation is done, the model provides an exact interpolation of the discrete elastic field. While less smooth than Shannon's, the new interpolation possesses a particular algebraic structure allowing one to reduce the strongly nonlocal problem to a nested set of analytically transparent second order differential equations.

The main novelty of the model is in its use of *several* deformation fields. One of the fields is the classical coarse grained field of continuum elasticity obtained by means of conventional scale free homogenization of the lattice field. The other fields correspond to the sub-continuum deformations which describe particular scales in the boundary layer structure of the typical solution of the discrete problem. We show that these length scales depend on the details of the interatomic potentials and may be vastly different from the apparent atomic scale. The resulting theory can be viewed either as local, with several deformation fields, or as a strongly nonlocal one, if all fields other than the macroscopic one are minimized out. Despite the strongly nonlocal appearance of the 'one-field' representation of the theory, which superficially resembles Kunin's quasicontinuum model [22], our nonlocal field can be decomposed into a number of sub-fields, solving a system of coupled second order linear differential equations.

Although we have chosen to present the main ideas in the simplest one-dimensional setting, the consideration is entirely general. To emphasize ideas, we limit our analysis to statics; the related issues of dynamics will be presented elsewhere.

The paper is organized as follows. In Sect. 2 we introduce the lattice model and solve by Fourier transform a generic discrete problem in the infinite domain. We show that the typical equilibrium displacement field exhibits a set of successively smaller internal length scales. The values of these scales depend on the location of the roots of the characteristic equation. We explicitly compute these roots for the special cases of lattices with next to nearest neighbor (NNN) and next to next to nearest neighbor (NNNN) interactions. In Sect. 3 we formulate our general approach which consists of four steps: (i) mapping the discrete problem into the Fourier space by a *discrete* Fourier transform; (ii) approximating the inverse of the Fourier image of the elasticity matrix (Green's function) in the Brillouin zone; (iii) expanding this approximation to the whole complex plane; and (iv) mapping the problem back into the physical space by a *continuous* Fourier transform. It is clear that the adequacy of a quasi-continuum model, obtained in this way, depends on the quality of the approximation for the Green's function. To illustrate this point we revisit in subsequent sections several existing approaches to this problem. We begin in Sect. 4 with Taylor expansions at long waves. Such expansions generate classical elasticity theory and its various strain gradient augmentations. In Sect. 5 we review the nonlocal continuum models aimed at exact interpolation of the discrete solution. We first recall the maximally smooth interpolation but then argue in favor of another, less smooth interpolation with a rational Fourier representation of the kernel. After truncation this Pad'e type interpolation scheme is used as a basis for a new multi-scale continuum theory developed in Sect. 6. Two modifications of the theory are presented, additive and multiplicative, but only the former is pursued in full detail. More specifically, in the remaining sections we present a case study of the additive version of the new theory adopted to the simplest nontrivial example of a lattice with nearest and next to nearest neighbor interactions (NNN chain). An infinite domain is treated in Sect. 7; the effects of external boundaries are discussed in Sect. 8. The final Sect. 9 contains our conclusions.

2 The discrete model

In this section we give a solution of a prototypical discrete problem which we later use as a benchmark to test various quasi-continuum approximations.

2.1 Formulation of the problem

Consider an infinite chain of interacting particles. Denote by x_k the coordinate of a particle with index k and by a—the characteristic interatomic distance. Assuming that the interactions are linear elastic, we can write the energy of the lattice in the form

$$W(x) = \frac{a}{4} \sum_{(k,q)\in\mathbb{Z}^2} \Psi_q \left[\frac{x_{k+q} - x_k}{a} - q\,\xi_q \right]^2 . \tag{1}$$

The energy depends on two types of parameters: the elastic moduli Ψ_q and the prestress ξ_q, both must satisfy the same symmetry constraints $\Psi_q = \Psi_{-q}$ and $\xi_q = \xi_{-q}$. For simplicity we additionally assume that the interactions have a finite range meaning that $\Psi_q = 0$ for $q > M$. We also impose on Ψ_q the conditions ensuring that the energy is positive definite (see below and [38]). If $\xi_q = \xi_p \neq 0$ the chain will be prestressed in the classical sense of continuum mechanics, if $\xi_q \neq \xi_p$ for some $q \neq p$ the chain will be prestressed microscopically, or hyper-prestressed [12].

To represent external loading we introduce a sequence of point forces f_k with appropriate rate of decay at infinity. We assume that the forces are balanced in the sense that

$$a \sum_{k\in\mathbb{Z}} f_k = 0. \tag{2}$$

The potential energy due to the forces f_k can be written in the form

$$P(x) = a \sum_{k\in\mathbb{Z}} f_k \left(x_k - x_k^o\right), \tag{3}$$

where the sequence x_k^o represents a reference configuration. Since in an infinite chain the hyper prestress can always be compensated by a system of distributed forces, we temporarily assume that for all q, $\xi_q = \xi$ and choose $x_k^o = \xi k a$. The effects of hyper-prestress will be illustrated in Sect. 8 where we deal with a finite chain.

By introducing the displacement field $u_k = x_k - x_k^o$ we can rewrite the elastic energy in the form

$$W(u) = \frac{a}{2} \sum_{k\in\mathbb{Z}} \sum_{q=-M}^{M} \Phi_q u_k \, u_{k+q}. \tag{4}$$

Here we defined the new set of elastic moduli: $a^2\Phi_q = a^2\Phi_{-q} = -\Psi_q$ for $q \neq 0$ and $a^2\Phi_0 = 2\sum_{q=1}^{M} \Psi_q$. In the new variables the system of equilibrium equations can be rewritten as a convolution

$$\sum_{q=-M}^{M} \Phi_q \; u_{k+q} = f_k. \tag{5}$$

We assume that the system (5) is supplemented by the appropriate growth conditions at infinity ensuring that the global force balance (2) follows necessarily.

2.2 Solution of the discrete problem

The system of equilibrium equations (5) can be solved by the discrete Fourier transform. We recall that a sequence y_k with at most polynomial growth can be mapped (in the sense of distributions) into the Fourier space by means of a transformation

$$y_{\mathcal{F}}(\lambda) = a \sum_{k\in\mathbb{Z}} y_k \, \mathrm{e}^{-ika\lambda}. \tag{6}$$

The function $y_{\mathcal{F}}(\lambda)$ is $2\pi a^{-1}$-periodic and is fully characterized by its restriction to the Brillouin zone

$$\mathbb{B} = \Big\{\lambda \in a^{-1}\mathbb{C} \; ; \; \Re e(\lambda) \in \big[-\pi/a, \pi/a\big]\Big\}. \tag{7}$$

To make the mapping $y_{\mathcal{F}}(\lambda)$ one-to-one it is usual to identify the lines $\Re e(\lambda) = \pm\pi/a$ which transforms the strip $\mathbb{B}$ into a cylinder. The inverse Fourier transform can then be defined by the formula

$$y_k = \frac{1}{2\pi} \int_{-\pi/a}^{\pi/a} y_{\mathcal{F}}(\lambda) \, \mathrm{e}^{ika\lambda} \, d\lambda, \tag{8}$$

where the integral is understood in the sense of Cauchy's principal value. The Fourier transform diagonalizes the system of equilibrium equations (5) and we can write

$$\Phi_{\mathcal{F}}(\lambda) \, u_{\mathcal{F}}(\lambda) = a f_{\mathcal{F}}(\lambda). \tag{9}$$

where $\Phi_{\mathcal{F}}(\lambda) = \Phi_{\mathcal{F}}(-\lambda)$ is the Fourier image of the elasticity "matrix"

$$\Phi_{\mathcal{F}}(\lambda) = a \sum_{k=-M}^{M} \Phi_k \mathrm{e}^{-i\lambda ka} = \frac{4}{a} \sum_{q=1}^{M} \Psi_q \sin^2\Big(\frac{\lambda q a}{2}\Big), \tag{10}$$

We can formally solve the system (9) and write the equilibrium displacement field as

$$u_{\mathcal{F}}(\lambda) = \big[\Phi_{\mathcal{F}}(\lambda)\big]^{-1} a f_{\mathcal{F}}(\lambda) \; + \; u^h_{\mathcal{F}}(\lambda). \tag{11}$$

where $u^h_{\mathcal{F}}(\lambda)$ is the Fourier image of the general solution of the homogeneous problem. To map solution (11) back into the physical space we need to perform the inverse Fourier transform (8). The result can be represented as

$$u_k = a \sum_{n\in\mathbb{Z}} G(k-n) f_n \; + \; u^h_k, \tag{12}$$

where $G(n)$ is the fundamental solution

$$G(n) = \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} \left[\Phi_{\mathcal{F}}(\lambda)\right]^{-1} \mathrm{e}^{ina\lambda}\, d\lambda, \tag{13}$$

and u_k^h is the general solution of the homogeneous system which can be written in the form

$$u_k^h = \sum_{p=0}^{\widehat{M}} C_p(k)\, \mathrm{e}^{ika\lambda_p}. \tag{14}$$

In (14) parameters λ_p with $p = 1, \ldots, \widehat{M}$ are the roots of the characteristic equation

$$\Phi_{\mathcal{F}}(\lambda) = 0, \tag{15}$$

which are located in $\mathbb{B}$ and C_p is a complex polynomial. The homogeneous solution can be specified by imposing kinematic conditions at infinity and we assume that these conditions require $u_k^h \equiv 0$. Therefore $G(n)$ is the Green's function of the problem. To compute the integral (13) one can use the method of residues and the first step is to evaluate the roots of the characteristic equation (15) in $\mathbb{B}$.

2.3 The characteristic equation

The function $\Phi_{\mathcal{F}}(\lambda)$ contains all the information about the elastic interactions in the system. In particular, the condition of elastic stability can be formulated in terms of $\Phi_{\mathcal{F}}(\lambda)$ as follows [22,38]

$$\Phi_{\mathcal{F}}(\lambda) > 0 \quad \text{for real } \lambda \notin 2\pi a^{-1}\mathbb{Z}. \tag{16}$$

In what follows we assume that this condition is satisfied which implies that the roots λ_p of $\Phi_{\mathcal{F}}(\lambda)$ are either complex or of the form $2\pi a^{-1}\mathbb{Z}$. In general, the function $\Phi_{\mathcal{F}}(\lambda)$ has a finite number of roots in any bounded region, in particular within the cylinder $\mathbb{B}$ the number of roots is assumed to be $2M$.

The generic roots appear either in doublets $(\lambda_p, -\lambda_p)$ with $\Re e(\lambda_p) = 0$ or $\Re e(\lambda_p) = \pi/a$, or in quadruplets $(\lambda_p, -\lambda_p, \bar{\lambda}_p, -\bar{\lambda}_p)$; outside $\mathbb{B}$ each root λ_p generates an infinite class of symmetric copies $\lambda_p + 2\pi a^{-1}\mathbb{Z}$. Due to the translational invariance of the system

$$\frac{d\Phi_{\mathcal{F}}}{d\lambda}(\lambda_0) = 2\sum_{q=1}^{M} q\, \Psi_q \sin\left(\lambda_0 q a\right) = 0,$$

and, therefore, there is always a non-generic double root $\lambda_0 = 0$. We assume that this trivial double root is not degenerate and that all the non-trivial roots are distinct. Following [22] we enumerate the roots within $\mathbb{B}$ in nondecreasing order of magnitude according to the rule

- $\lambda_0 = \lambda_1 = 0$;
- $\lambda_{2m} = -\lambda_{2m+1}$, with $\Im m(\lambda_{2m}) > 0$ $(m \geq 1)$.

To illustrate these assumptions we consider the simplest examples. Thus, if only the nearest neighbors are interacting (NN model), the nontrivial roots are absent which makes this case degenerate. If next to nearest neighbor interactions are also taken into account (NNN model), and the lattice is stable, the trivial double root is supplemented by either a pair of purely imaginary roots $(\lambda_p, -\lambda_p)$ with $\Re e(\lambda_p) = 0$, or by a pseudo-quadruplet $(\lambda_p, -\lambda_p, \bar{\lambda}_p, -\bar{\lambda}_p)$ with $\Re e(\lambda_p) = \pm\pi/a$ which reduces to a pair $(\lambda_p, -\lambda_p)$ if $\mathbb{B}$ is viewed as a cylinder [12]. The generic quadruplets do not appear till the interaction of the third nearest neighbors is taken into consideration (NNNN model) as we briefly show in the Appendix A (see also [38]).

Due to the symmetry of the roots of the characteristic equation, it is always possible to choose the closed integration path around the poles in (13) differently for $n > 0$ and $n < 0$ so that symmetric poles λ_{2m} and

λ_{2m+1} within $\mathbb{B}$ contribute jointly to produce terms like $e^{i\lambda_{2m}|n|a}$. We can then write the Green's function in (13) as a sum

$$G(n) = G_c(n) + \sum_{m=1}^{\widehat{M}} G_m(n), \tag{17}$$

where the first term

$$G_c(n) = -\frac{|n|a}{2K}, \tag{18}$$

representing the main contribution to the asymptotics at infinity, is due to the trivial double root of equation (15). It represents the discrete analog of a Green's function in classical elasticity. The parameter

$$K = \frac{1}{2a}\frac{d^2\Phi_{\mathcal{F}}}{d\lambda^2}(0) = \sum_{q=1}^{M} q^2\ \Psi_q \tag{19}$$

is then equal to homogenized elastic modulus. The other additive contributions to the Green's function are due to nontrivial roots of the characteristic equation. For instance, a generic couple of roots λ_{2m} and λ_{2m+1} produce a term

$$G_m(n) = \frac{i\,e^{i\lambda_{2m}|n|a}}{\Phi'_{\mathcal{F}}(\lambda_{2m})}. \tag{20}$$

The corresponding functions in the physical space decay exponentially at the distance of the order of the radius of effective interactions λ_{2m}^{-1}. The main nonlocal contribution of this type is due to the shallowest exponent corresponding to the first nontrivial roots of the function $\Phi_{\mathcal{F}}(\lambda)$.

Notice that the functions (20) are complex except when the roots λ_{2m} are purely imaginary. In order to rewrite the Green's function as a sum of real contributions, we can use the fact that the roots with $\Re e(\lambda_{2m}) \neq 0$ appear in symmetric quadruplets. The corresponding additive terms can then be organized in pairs and we can write

$$\hat{G}_m(n) = \Re e\Big(\frac{i\,e^{i\lambda_{2m}|n|a}}{\Phi'_{\mathcal{F}}(\lambda_{2m})}\Big) \equiv \frac{1}{2}\left[\frac{i\,e^{i\lambda_{2m}|n|a}}{\Phi'_{\mathcal{F}}(\lambda_{2m})} + \frac{i\,e^{-i\bar{\lambda}_{2m}|n|a}}{\Phi'_{\mathcal{F}}(-\bar{\lambda}_{2m})}\right]. \tag{21}$$

Here we have used that $\Phi'_{\mathcal{F}}\big(-\overline{\lambda_p}\big) = -\overline{\Phi'_{\mathcal{F}}(\lambda_p)}$. The terms (21) represent oscillatory corrections to the equilibrium displacement field which decay on average exponentially at the scale $|\lambda_{2m}|^{-1}$. The adjustment of the formula (21) to the case of pseudo-quadrouplets with $\Re(\lambda_{2m}) = \pm\pi/a$, when oscillations are binary, is straightforward.

3 Continuum and quasi-continuum approximations

In order to obtain a continuum analog of the discrete theory, one has to replace the discrete sequence u_k representing a response of the system to the given loads f_k by a continuous function $u(s)$ of the spatial variable $s \in \mathbb{R}$. This function must be selected to ensure that $u(ka)$ is close to u_k; for instance $u(s)$ may be a continuous interpolation for u_k. The problem of building a continuum approximation includes the task of finding the set of equations which generate the function $u(s)$ as an equilibrium displacement field when the applied loads f_k are replaced by a continuous function $f(s)$ approximating these discrete loads. It is desirable that the approximate continuum theory preserves the variational nature of the discrete theory, therefore, it is also necessary to find the expression for the energy functional which is minimized by $u(s)$.

The solution of the imprecise problem formulated above is obviously non unique and in what follows we adopt a particular strategy which is suggested by the classical homogenization theory. In very general terms we shall attempt to approximate the Green's function of the original problem in the Fourier space. The first

step is then to map the original discrete problem into the Fourier space by using the discrete Fourier transform (6). The second step is to replace the exact equation in the Fourier space (9) by an approximate equation

$$\Phi^*_{\mathcal{F}}(\lambda)\, u^*_{\mathcal{F}}(\lambda) = a f^*_{\mathcal{F}}(\lambda). \tag{22}$$

Here the new functions $\Phi^*_{\mathcal{F}}(\lambda)$ and $f^*_{\mathcal{F}}(\lambda)$, defined on the whole complex plane, substitute the functions $\Phi_{\mathcal{F}}(\lambda)$ and $f_{\mathcal{F}}(\lambda)$ defined on $\mathbb{B}$. If these functions are chosen appropriately, the solution $u^*_{\mathcal{F}}(\lambda)$ of (22), which is now defined on the whole complex plane, approximates the discrete solution $u_{\mathcal{F}}(\lambda)$. After the function $u^*_{\mathcal{F}}(\lambda)$ is recovered from (22) the continuum displacement field is furnished by the continuum inverse Fourier transform

$$u(s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} u^*_{\mathcal{F}}(\lambda)\, \mathrm{e}^{is\lambda}\, d\lambda. \tag{23}$$

The continuum equations can be recovered from

$$u(s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} a\, [\Phi^*{}_{\mathcal{F}}(\lambda)]^{-1} f^*_{\mathcal{F}}(\lambda)\, e^{i\lambda s} d\lambda = \int_{-\infty}^{\infty} G^*(s-\hat{s})\, f(\hat{s})\, d\hat{s}. \tag{24}$$

where the Green's function is defined as the continuum inverse Fourier transform of $\Phi^*{}_{\mathcal{F}}(\lambda)$

$$G^*(s) = \frac{a}{2\pi} \int_{-\infty}^{\infty} [\Phi^*{}_{\mathcal{F}}(\lambda)]^{-1} e^{i\lambda s} d\lambda. \tag{25}$$

The continuum approximation for the force distribution can be computed from

$$f(s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f^*_{\mathcal{F}}(\lambda)\, e^{i\lambda s} d\lambda. \tag{26}$$

The variational structure of the problem is obviously preserved by the above procedure.

The main problem, which will mostly occupy us in what follows, is how to substitute the function $\Phi_{\mathcal{F}}(\lambda)$ by a new function $\Phi^*_{\mathcal{F}}(\lambda)$. Parallel approximations should be also developed for the function $f_{\mathcal{F}}(\lambda)$.

Despite its generality, the above algorithm allows one to deal with problems on the infinite domain only. To formulate the associated continuum problem on a finite domain, one has to derive an additional set of boundary conditions, reflecting the presence of microscopic forces at the boundary. We shall address this issue in Sect. 8 for a particular lattice model.

4 Polynomial models

In this section we discuss three continuum theories based on the polynomial approximation of the elasticity operator (rather than its inverse) in the Fourier space. The first approximate model of this type is the classical elasticity. The second model is the strain gradient elasticity theory based on the Taylor expansion (at long waves) of the function $\Phi_{\mathcal{F}}(\lambda)$ going beyond the classical quadratic term. The third approximation is a gradient elasticity theory, which is based on a multi-point Taylor expansion of $\Phi_{\mathcal{F}}(\lambda)$ which uses information about both the long and the short wave structure of the discrete elasticity operator.

4.1 Classical elasticity

To obtain the classical elasticity theory we need to perform the Taylor's expansion of the function $\Phi_{\mathcal{F}}(\lambda)$ near the origin. We obtain

$$\Phi_{\mathcal{F}}(\lambda) = \sum_{q=1}^{\infty} \frac{\lambda^{2q}}{(2q)!} \frac{d^{2q}\Phi_{\mathcal{F}}}{d\lambda^{2q}}(0). \tag{27}$$

By preserving only the first term we can write

$$\Phi^*_{\mathcal{F}}(\lambda) = Ka\lambda^2 = \Phi^*_c(\lambda). \tag{28}$$

One can see that the resulting theory captures only the trivial double root of the characteristic equation at $\lambda = 0$. The implicit assumption here that justifies the truncation of the infinite Taylor's series is that the external parameter with the scale of length, represented here by λ^{-1}, is much larger than the internal length scale a. It is essentially assumed that the interpolating field $x(s)$ is sufficiently smooth in the sense that the reference atomic length a is much smaller than the characteristic length of variations of $x(s)$.

Given (28) we can apply the inverse transform (23) to (22) and obtain

$$-K\big[D^2 u_c(s)\big] = f(s), \tag{29}$$

where K is given in (19) and $D = d/ds$. The formal solution of the Eq. (29) can be written in the form

$$u_c(s) = \int_{-\infty}^{\infty} G^*_c(s-\check{s}) f(\check{s}) d\check{s} \tag{30}$$

where

$$G^*_c(s) = \frac{a}{2\pi} \int_{-\infty}^{\infty} [\Phi^*_{\mathcal{F}}(\lambda)]^{-1} e^{i\lambda s} d\lambda = -\frac{|s|}{2K}, \tag{31}$$

is the classical Green's function which interpolates the corresponding coarse term in the discrete solution (18) in the sense that $G^*_c(na) = G_c(n)$. The continuum energy generating the equilibrium equations (29) is

$$W_c(u_c) = \frac{K}{2} \int_{-\infty}^{\infty} \big[Du_c(s)\big]^2 ds. \tag{32}$$

One can see that in this approximation we are losing information about the "microscopic" corrections to the coarse grained displacement field described by (20). In particular, we miss the exponential boundary layers around the points of application of the concentrated forces.

Although the resulting model does not contain an internal length scale and can, in principle, be used at all scales, it is expected to be adequate only at the scales much larger than $|\lambda_2|^{-1}$, where λ_2 is the closest to the origin non-trivial root of the characteristic equation. One can conclude that the classical approximation should be particularly effective when there are no non-trivial roots close to the origin. It is then not surprising that it gives an exact interpolation of the discrete fields for the NN model (see also [11]).

4.2 Strain-gradient elasticity

To go beyond the classical continuum elasticity one can approximate the Fourier symbol of the discrete operator by the higher order Taylor's expansion around the point $\lambda = 0$ (e.g. [8]). This again implies long-wave approximation and requires $|\lambda a| \ll 1$. By expanding $\Phi_{\mathcal{F}}(\lambda)$ up to order $M^* \geq 1$ we obtain

$$\Phi^*_{\mathcal{F}}(\lambda) = Ka\lambda^2 \mathcal{P}_{M^*}(\lambda^2), \tag{33}$$

where

$$\mathcal{P}_{M^*}(z) = \sum_{q=1}^{M^*} \frac{z^{q-1}}{Ka(2q)!} \frac{d^{2q}\Phi_{\mathcal{F}}}{d\lambda^{2q}}(0).$$

If we extend the definition of the function $\Phi^*_{\mathcal{F}}(\lambda)$ in (33) from $\mathbb{B}$ to the whole complex plane, we obtain in the real space the following equilibrium equation

$$-KD^2 \mathcal{P}_{M^*}(-D^2) u(s) = f(s). \tag{34}$$

The corresponding energy function reads

$$W^*(u) = \frac{K}{2}\int_{-\infty}^{\infty}\left\{\sum_{q=1}^{M^*}\frac{(-1)^{q-1}}{Ka(2q)!}\frac{d^{2q}\Phi_{\mathcal{F}}}{d\lambda^{2q}}(0)\left[D^q u(s)\right]^2\right\}ds. \tag{35}$$

To illustrate this approximation, consider the simplest case when the polynomial $\mathcal{P}_{M^*}$ is of the second order

$$\Phi^*_{\mathcal{F}}(\lambda) = Ka\lambda^2\Big[1-\frac{\lambda^2}{(\lambda^*_2)^2}\Big], \tag{36}$$

where

$$(\lambda^*_2)^{-2} = a^2\frac{\sum_{q=1}^{M} q^4\Psi_q}{12\sum_{q=1}^{M} q^2\Psi_q}. \tag{37}$$

The equilibrium equation can then be written as

$$-K\left[D^2\left(1+\frac{1}{\lambda^{*2}_2}D^2\right)u(s)\right] = f(s). \tag{38}$$

and the elastic energy takes the form

$$W^*(u) = \frac{K}{2}\int_{-\infty}^{\infty}\left\{\left[Du(s)\right]^2 - \frac{1}{\lambda^{*2}_2}\left[D^2u(s)\right]^2\right\}ds. \tag{39}$$

The associated Green's function contains both the coarse grained classical contribution and the microscopic correction

$$G^*(s) = \frac{a}{2\pi}\int_{-\infty}^{\infty}[\Phi^*_{\mathcal{F}}(\lambda)]^{-1}e^{i\lambda s}d\lambda = -\frac{1}{K}\left[\frac{|s|}{2}+\Im m\left(\frac{1}{\lambda^*_2}\mathrm{e}^{i\lambda^*_2|s|}\right)\right]. \tag{40}$$

Since we are interested in the case when the ensuing model is stable, we assume that the parameter λ^*_2 is purely imaginary. It is well known that this puts restrictions on the elastic moduli which are not realistic for many materials (e.g. [38]). Moreover, in view of (37), the condition $|\lambda^*_2 a| \ll 1$ means that for this approximation to work, the "homogenized" modulus K defined in (19) must be small

$$\frac{|K|}{|\sum_{q=1}^{M} q^4\Psi_q|} \ll 1,$$

which means that the higher gradient terms are relevant only in the domain of parameters where the homogenized theory exhibits *softening*.

4.3 Gradient approximation by first roots

To construct a low order polynomial approximation for the function $\Phi_{\mathcal{F}}(\lambda)$ which captures the actual root λ_2 of the characteristic equation in $\mathbb{B}$, one can use a two-point (or multi-point) expansion [22,34]. This approximation can be obtained from the Weierstrass factorization of the function $\Phi_{\mathcal{F}}(\lambda)$

$$\Phi_{\mathcal{F}}(\lambda) = Ka\lambda^2\prod_{m=1}^{\infty}\left[1-\frac{\lambda^2}{\lambda^2_{2m}}\right]. \tag{41}$$

To construct the first gradient approximation of this type in the generic case when $\Re e(\lambda_2) \neq 0$, we need to truncate the expansion (41) and preserve only the first four symmetric roots of the characteristic equation that are the closest to the origin. By isolating these roots we can write

$$\Phi^*_{\mathcal{F}}(\lambda) = Ka\lambda^2\left[1-\frac{\lambda^2}{\lambda_2^2}\right]\left[1-\frac{\lambda^2}{\bar{\lambda}_2^2}\right]. \tag{42}$$

If we now extend this new function $\Phi^*_{\mathcal{F}}(\lambda)$ from $\mathbb{B}$ to the whole complex plane we obtain in the physical space the following equilibrium equation

$$-K\left[D^2\left(1+\frac{1}{\lambda_2{}^2}D^2\right)\left(1+\frac{1}{\bar{\lambda}_2{}^2}D^2\right)u(s)\right] = f(s). \tag{43}$$

The continuum elastic energy corresponding to (43) takes the form

$$W^*(u) = \frac{K}{2}\int\left\{\left[Du(s)\right]^2 - \frac{2\Re e(\lambda_2^2)}{|\lambda_2^2|^2}\left[D^2u(s)\right]^2 + \frac{1}{|\lambda_2^2|^2}\left[D^3u(s)\right]^2\right\}ds. \tag{44}$$

As in the preceding section we can write explicitly the Green's function for the resulting theory (see also [22])

$$G^*(s) = -\frac{1}{K}\left[\frac{|s|}{2} + \Im m\left(\frac{\bar{\lambda}_2^2}{(\lambda_2^2-\bar{\lambda}_2^2)\lambda_2}e^{i\lambda_2|s|}\right)\right]. \tag{45}$$

The simplest gradient theory of this type emerges in the (generic) case when $\Re e(\lambda_2) = 0$. Then the first nontrivial roots of the characteristic equation are purely imaginary (as, for instance, in the NNN model) and the Fourier image of the elasticity operator $\Phi_{\mathcal{F}}(\lambda)$ can be approximated by

$$\Phi^*_{\mathcal{F}}(\lambda) = Ka\lambda^2\left[1-\frac{\lambda^2}{\lambda_2^2}\right]. \tag{46}$$

The equilibrium equation have the same general structure as in (38)

$$-K\left[D^2\left(1+\frac{1}{\lambda_2{}^2}D^2\right)u(s)\right] = f(s), \tag{47}$$

modulo the replacement of the approximate scale $(\lambda_2^*)^{-1}$ by the physical scale λ_2^{-1}. The elastic energy takes the familiar form

$$W^*(u) = \frac{K}{2}\int_{-\infty}^{\infty}\left\{\left[Du(s)\right]^2 - \frac{1}{\lambda_2^2}\left[D^2u(s)\right]^2\right\}ds. \tag{48}$$

For this model to be applicable, the function $u(s)$ must be sufficiently smooth in the sense that $|\lambda| \ll |\lambda_4| \equiv \min_{m\geq 2}\{|\lambda_{2m}|\}$; we also have an additional implicit restriction on the microscopic elastic moduli in the form $|\lambda_2| \ll |\lambda_4|$.

In general, the advantage of the successive "multi-point" polynomial approximations by the first roots is that they allow one to link the order of the resulting PDE to the particular physical length scales, which the theory attempts to capture. The problem is that the desire to increase the precision of this type of theories may require resolution of the derivatives of prohibitively high order.

5 Interpolation schemes

The polynomial methods discussed in the previous section capture only sufficiently smooth, long wave structure of the discrete solution of the equilibrium equations and in all these approaches an important information about the micro-field is necessarily lost. To recover this information one can try instead of approximating, to interpolate the discrete solution and formulate the continuum theory for the interpolating function. The interpolation problem has multiple solutions and below we discuss two different approaches. The first approach is based on the idea of maximally smooth interpolation. The second approach provides less smooth interpolation, but maintains a simple algebraic structure of the theory and is compatible with a much broader class of functions. The truncation of the series appearing in the second approach will be essential for the formulation of our multi-scale quasicontinuum theory in Sect. 6.

5.1 Smooth interpolation

Instead of expanding the function $\Phi_{\mathcal{F}}(\lambda)$ at small $|\lambda|$ one can follow the original idea of Shannon, which was adopted to crystal elasticity in [21,22,34], and preserve the exact equation (9) everywhere on $\mathbb{B}$. To expand (22) onto the whole complex plane we need to introduce the new functions

$$u^*_{\mathcal{F}}(\lambda) = 1_{\mathbb{B}}(\lambda) u_{\mathcal{F}}(\lambda), \quad \Phi^*_{\mathcal{F}}(\lambda) = 1_{\mathbb{B}}(\lambda)\Phi_{\mathcal{F}}(\lambda) \quad \text{and} \quad f^*_{\mathcal{F}}(\lambda) = 1_{\mathbb{B}}(\lambda) f_{\mathcal{F}}(\lambda), \tag{49}$$

where

$$1_{\mathbb{B}}(\lambda) = \begin{cases} 1, \text{ if } \lambda \in \mathbb{B} \\ 0, \text{ otherwise} \end{cases} \tag{50}$$

is the indicator function of the domain $\mathbb{B}$, and recall that in the physical space the function $y^*_{\mathcal{F}}(\lambda) = 1_{\mathbb{B}}(\lambda)\, y_{\mathcal{F}}(\lambda)$ can be presented as

$$y(s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} y^*_{\mathcal{F}}(\lambda)\, \mathrm{e}^{is\lambda}\, d\lambda = \sum_{k\in\mathbb{Z}} y_k \operatorname{sinc}\left(\frac{s}{a} - k\right). \tag{51}$$

where

$$\operatorname{sinc}(t) = \frac{\sin(\pi t)}{\pi t}.$$

If we now use the transform (51) to bring the Eq. (22) back into the real space, we obtain a nonlocal problem

$$\int_{-\infty}^{\infty} \mathcal{L}\left(\frac{s-\check{s}}{a}\right) u(\check{s})\, d\check{s} = f(s) \tag{52}$$

where the kernel is

$$\mathcal{L}(t) = \sum_{q=-M}^{M} \frac{\Phi_q}{a} \operatorname{sinc}\big(t-q\big) \;\equiv\; 2\operatorname{sinc}(t) \sum_{q=1}^{M} \frac{\Psi_q}{a^3} \left\{ \frac{\big[1-(-1)^q\big]t^2 - q^2}{t^2 - q^2} \right\}. \tag{53}$$

The corresponding elastic energy can be written as

$$W(u) = \frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathcal{L}\left(\frac{s-\check{s}}{a}\right) u(s)\, u(\check{s})\, ds\, d\check{s}. \tag{54}$$

On the class of functions whose Fourier transform is supported in $\mathbb{B}$, the continuum energy (54) is identical to the discrete one (4). In particular, if discrete theory is stable, the continuum theory is stable as well.

While this form of interpolation, known also as a quasi-continuum theory (see [22]), is optimal in terms of the smoothness of the approximation, it leads to analytically opaque strongly nonlocal problems, restricted to test-functions with $\mathbb{B}$-band-limited spectrum. The resulting integral equilibrium equation is exactly as complex to handle as the infinite system of equations in the original discrete theory and therefore the theory has not yet found sufficiently broad applications. The relation of this nonlocal model to the coarse classical continuum model is not explicit and therefore the quasi-continuum interpolation has not become a source of useful non-classical corrections.

5.2 Padé interpolation

One can obviously come up with many other interpolation schemes, which are necessarily less smooth than the Shannon's interpolation. Among these interpolations, however, one can try to find the one with a desired algebraic structure. To see which structure may be beneficial we first consider a restriction of the standard Mittag–Leffler's fractional decomposition [20] for the function $\big[\Phi_{\mathcal{F}}(\lambda)\big]^{-1}$ to the domain $\mathbb{B}$. The approximating operator is then

$$\big[\Phi^*_{\mathcal{F}}(\lambda)\big]^{-1} = \frac{1}{Ka\lambda^2} + 2\sum_{m=1}^{\widehat{M}} \frac{\lambda_{2m}}{\Phi'_{\mathcal{F}}(\lambda_{2m})}\frac{1}{\lambda^2-\lambda^2_{2m}} \tag{55}$$

where $\widehat{M}$ is the number of nonzero symmetric couples of the roots $(\lambda_{2m}, -\lambda_{2m})$ of (15) in $\mathbb{B}$ (the factor 2 in (55) has to be omitted if $\Re e(\lambda_{2m}) = \pm\pi/a$). This rational approximation ensures that

$$\int_{-\infty}^{\infty} \big[\Phi^*_{\mathcal{F}}(\lambda)\big]^{-1} \mathrm{e}^{i\lambda ka}\, d\lambda = \int_{-\pi/a}^{\pi/a} \big[\Phi_{\mathcal{F}}(\lambda)\big]^{-1} \mathrm{e}^{i\lambda ka}\, d\lambda. \tag{56}$$

An important observation is that in this approximation $G^*(na) \equiv G(n)$ which is necessary for the exact interpolation of the discrete solution of the equilibrium equations. One can also see that the approximate continuum Fourier symbol $\Phi^*_{\mathcal{F}}(\lambda)$ is equal to the discrete one $\Phi_{\mathcal{F}}(\lambda)$ only in the weak sense of (56) while in the maximally smooth approximation (49_2) the two symbols agree in the interior of $\mathbb{B}$ pointwise. Contrary to $\Phi_{\mathcal{F}}(\lambda)$ the function $\Phi^*_{\mathcal{F}}(\lambda)$ has only finite number of roots in the complex plane, however, now it also has a finite number of poles.

The ensuing continuum theory is again strongly nonlocal. In particular, the equilibrium equation can be written in the form

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \Phi^*_{\mathcal{F}}(\lambda)\, u_{\mathcal{F}}(\lambda)\, \mathrm{e}^{i\lambda s}\, d\lambda = af(s), \tag{57}$$

where

$$\Phi^*_{\mathcal{F}}(\lambda) = Ka\lambda^2\left\{1 + \frac{2\sum_{m=1}^{\widehat{M}} \frac{Ka\lambda^2}{\lambda_{2m}\Phi'_{\mathcal{F}}(\lambda_{2m})}\prod_{\substack{p=1\\p\neq m}}^{\widehat{M}}\big(1-\frac{\lambda^2}{\lambda^2_{2p}}\big)}{\prod_{q=1}^{\widehat{M}}\big(1-\frac{\lambda^2}{\lambda^2_{2q}}\big) - 2\sum_{m=1}^{\widehat{M}} \frac{Ka\lambda^2}{\lambda_{2m}\Phi'_{\mathcal{F}}(\lambda_{2m})}\prod_{\substack{p=1\\p\neq m}}^{\widehat{M}}\big(1-\frac{\lambda^2}{\lambda^2_{2p}}\big)}\right\}. \tag{58}$$

In the physical space the Eq. (57) takes the form

$$-D\int_{-\infty}^{\infty} \mathcal{K}(s-\check{s})\, Du(\check{s})\, d\check{s} = f(s) \tag{59}$$

where the kernel is

$$\mathcal{K}(s) = K\left\{\delta(s) + \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{2\sum_{m=1}^{\widehat{M}} \frac{Ka\lambda^2}{\lambda_{2m}\Phi'_{\mathcal{F}}(\lambda_{2m})}\prod_{\substack{p=1\\p\neq m}}^{\widehat{M}}\big(1-\frac{\lambda^2}{\lambda^2_{2p}}\big)\,\mathrm{e}^{i\lambda s}}{\prod_{q=1}^{\widehat{M}}\big(1-\frac{\lambda^2}{\lambda^2_{2q}}\big) - 2\sum_{m=1}^{\widehat{M}} \frac{Ka\lambda^2}{\lambda_{2m}\Phi'_{\mathcal{F}}(\lambda_{2m})}\prod_{\substack{p=1\\p\neq m}}^{\widehat{M}}\big(1-\frac{\lambda^2}{\lambda^2_{2p}}\big)}\, d\lambda\right\}. \tag{60}$$

One can see that the Dirac's delta in (60) corresponds to classical elasticity, while the remaining strongly nonlocal contribution is due to the effects of discreteness. The model has a variational structure with the elastic energy given by

$$W^*(u) \equiv \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathcal{K}(s-\check{s})\big[Du(s)\big]\big[Du(\check{s})\big]\, ds\, d\check{s}. \tag{61}$$

By using Parseval's identity, one can show that if the discrete model is stable then the energy (61) is positive definite on all displacement fields excluding translations and has the same minimal value as the discrete energy (4).

6 Multi-scale continuum theory

In this section we show that despite its nonlocal appearance, the truncated Padé interpolation introduced in the previous section has an equivalent local formulation. Moreover we propose two different local formulations based on either additive or multiplicative decomposition of the inverse elasticity operator $\left[\Phi^*_{\mathcal{F}}(\lambda)\right]^{-1}$. The detailed structure of the 'additive' version of the theory will be illustrated by examples in the succeeding Sections while the detailed study of the 'multiplicative' version will be left for future work.

6.1 Additive decomposition

Behind the additive model is the following rewriting of the formula (55)

$$\left[\Phi^*_{\mathcal{F}}(\lambda)\right]^{-1} = \left[(\Phi^*_c)_{\mathcal{F}}(\lambda)\right]^{-1} + \sum_{m=1}^{\widehat{M}} \left[(\Phi^*_m)_{\mathcal{F}}(\lambda)\right]^{-1}. \tag{62}$$

Here the classical coarse contribution $\Phi^*_c(\lambda)$ given by (28) is written separately. The additive microscopic corrections, coming from the nontrivial roots of the characteristic equation, are of the form

$$(\Phi^*_m)_{\mathcal{F}}(\lambda) = \frac{\Phi'_{\mathcal{F}}(\lambda_{2m})}{\lambda_{2m}}(\lambda^2 - \lambda^2_{2m}). \tag{63}$$

The main observation is that this representation for the Green's function implies the following additive decomposition for the displacement field

$$u(s) = u_c(s) + \sum_{m=1}^{\widehat{M}} u^*_m(s). \tag{64}$$

Here, again, $u_c(s)$ is the solution of the coarse (homogenized) equation (29), while $u^*_m(s)$ are the microscopic corrections linked to the corresponding roots of the characteristic equation. We can write

$$u^*_m(s) = \int_{-\infty}^{\infty} G^*_m(s - \hat{s})\, f(\hat{s})\, d\hat{s}. \tag{65}$$

where the microscopic Green's function associated with the roots $\pm\lambda_{2m}$ is

$$G^*_m(s) = \frac{a}{2\pi} \int_{-\infty}^{\infty} [(\Phi^*_m)_{\mathcal{F}}(\lambda)]^{-1}\, \mathrm{e}^{i\lambda s}\, d\lambda = -\lambda_{2m} \frac{i\mathrm{e}^{i\lambda_{2m}|s|}}{2K\kappa_{2m}}. \tag{66}$$

Here we defined

$$\kappa_{2m} = -\frac{\Phi'_{\mathcal{F}}(\lambda_{2m})}{2Ka\lambda_{2m}} = -\frac{1}{K}\sum_{q=1}^{\widehat{M}} q\, \Psi_q \frac{\sin(\lambda_{2m} q a)}{\lambda_{2m} a}. \tag{67}$$

To understand the meaning of the fields $u^*_m(s)$ it is instructive to rewrite the corresponding individual equilibrium equations in the Fourier space

$$(u^*_m)_{\mathcal{F}}(\lambda) = -\frac{1}{\kappa_{2m} K} \frac{f_{\mathcal{F}}(\lambda)}{\lambda^2 - \lambda^2_{2m}}. \tag{68}$$

By performing inverse Fourier transform we obtain in the physical space

$$\kappa_{2m} K \left[D^2 u_m^*(s) + \lambda_{2m}^2 u_m^*(s) \right] = f(s). \tag{69}$$

One can see that the micro-components of the continuum field $u_m^*(s)$ satisfy simple Helmholtz-type equations and each individual micro-problem have a standard variational structure with the energy

$$W_m(u_m^*) \sim \frac{\kappa_{2m} K}{2} \int_{-\infty}^{\infty} \left\{ \left[D u_m^*(s) \right]^2 - \lambda_{2m}^2 \left[u_m^*(s) \right]^2 \right\} ds. \tag{70}$$

These variational problems are not translation invariant because we deal here only with differences of the displacement fields.

Notice that the fields $u_m^*(s)$ and $u_{m+1}^*(s)$ are complex and conjugate when the associated roots of the characteristic equation $(\lambda_{2m}, \lambda_{2m+1} = -\lambda_{2m})$ and $(\lambda_{2m+2} = \overline{\lambda_{2m}}, \lambda_{2m+3} = -\overline{\lambda_{2m}})$ form a quadruplet with $\Re e(\lambda_{2m}) \neq 0$. In this case only the sum $u_m^*(s) + u_{m+1}^*(s)$ is real. To find this real field one can represent (69) as a coupled system of two differential equations for the real and imaginary parts of $u_m^*(s)$. An alternative way is to deal directly with all four roots representing the quadruplet, which leads to a nonlocal formulation for the real function $u_m^{**}(s) = [u_m^*(s) + \overline{u_m^*}(s)]/2$, as detailed in Appendix B.

Despite their apparent independence, the fields u_c and u_m^* are coupled through the nonlocal relations that can be obtained by eliminating the applied loads $f(s)$ from the individual equations (29) and (69). Indeed, we have

$$(u_m^*)_{\mathcal{F}}(\lambda) = -\frac{1}{\kappa_{2m}} \frac{\lambda^2}{\lambda^2 - \lambda_{2m}^2} (u_c)_{\mathcal{F}}(\lambda). \tag{71}$$

In the physical space, this gives for each u_m^* a Helmholtz equation with 1D Laplacian of the macroscopic field u_c in the right hand side. This in turn implies a nonlocal relation between $u_m^*(s)$ and $u_c(s)$ of the type

$$u_m^*(s) \equiv -K \int_{-\infty}^{\infty} G_m^*(s - \check{s}) D^2 u_c(\check{s})\, d\check{s}. \tag{72}$$

We may conclude that after the classical solution is found, the microscopic corrections can be reconstructed by means of a straightforward nonlocal filtering of the coarse field with an exponential kernel. The computation of the microscopic fields at increasingly smaller scales can also be arranged as a nested process when the field at a larger scale defines the one at a smaller scale. The full nonlocal structure of the original problem (59) is recovered if all microfields are minimized out and the problem is formulated directly in terms of the total displacement field $u(s)$.

While the complete expansion (62) provides an exact continuum interpolation of the discrete solution, in the case when only the first roots of the characteristic equation in $\mathbb{B}$ are retained, the truncated expansions of the type (62) generate a sequence of approximate multi-scale continuum models whose accuracy is the function on the number of internal scales retained.

6.2 Multiplicative decomposition

An alternative multi-field representation of the same model is based on the following rewriting of the formula (55)

$$\Phi_{\mathcal{F}}^*(\lambda) = \widehat{\Phi}_{\mathcal{F}}(\lambda) \left[\widetilde{\Phi}_{\mathcal{F}}(\lambda) \right]^{-1} \tag{73}$$

where

$$\widehat{\Phi}_{\mathcal{F}}(\lambda) = K a \lambda^2 \prod_{q=1}^{\widehat{M}} \left(1 - \frac{\lambda^2}{\lambda_{2q}^2} \right) \tag{74}$$

and

$$\widetilde{\Phi}_{\mathcal{F}}(\lambda) = \prod_{q=1}^{\widehat{M}} \left(1 - \frac{\lambda^2}{\lambda_{2q}^2}\right) - 2 \sum_{m=1}^{\widehat{M}} \frac{Ka\lambda^2}{\lambda_{2m} \Phi'_{\mathcal{F}}(\lambda_{2m})} \prod_{\substack{p=1 \\ p \neq m}}^{\widehat{M}} \left(1 - \frac{\lambda^2}{\lambda_{2p}^2}\right), \tag{75}$$

are both positive definite. The multiplicative decomposition (73) suggests that we can introduce a meso-scopic field $\hat{u}(s)$ which satisfies the equation

$$\widehat{\Phi}_{\mathcal{F}}(\lambda) \hat{u}_{\mathcal{F}}(\lambda) = f_{\mathcal{F}}(\lambda). \tag{76}$$

Observe that this field is different from the classical macroscopic field $u_c(s)$ and is instead a solution of the gradient theory based on Taylor approximation by $\widehat{M}$ first roots (see Sect. 4.3). The meso-scopic equilibrium equation can be written in the physical space as

$$-K \left[D^2 \prod_{q=1}^{\widehat{M}} \left(1 + \frac{D^2}{\lambda_{2q}^2}\right) \hat{u}(s) \right] = f(s). \tag{77}$$

The field $\hat{u}(s)$ is related to the microscopic (interpolating) field $u(s)$ by the following equation

$$u_{\mathcal{F}}(\lambda) = \widetilde{\Phi}_{\mathcal{F}}(\lambda) \hat{u}_{\mathcal{F}}(\lambda), \tag{78}$$

where $u_{\mathcal{F}}(\lambda)$ is the continuous Fourier transform of the microscopic field $u(s)$ (we consider infinite domain with zero boundary conditions). In the physical space we obtain

$$u(s) = \left[\prod_{q=1}^{\widehat{M}} \left(1 + \frac{D^2}{\lambda_{2q}^2}\right) + 2 \sum_{m=1}^{\widehat{M}} \frac{KaD^2}{\lambda_{2m} \Phi'_{\mathcal{F}}(\lambda_{2m})} \prod_{\substack{p=1 \\ p \neq m}}^{\widehat{M}} \left(1 + \frac{D^2}{\lambda_{2p}^2}\right) \right] \hat{u}(s). \tag{79}$$

The inversion of this equation generates a kernel providing the smoothing (coarse-graining) of the micro-scopic field $u(s)$ at the meso-scopic level.

The polynomial structure of the operator in (79) suggests that in addition to micro and meso-scopic fields, one can introduce a set of natural intermediate-scale corrections that can be resolved in the sequential order. If we denote by $\widetilde{M} \leq \widehat{M}$ the order of the polynomial (75) with respect to λ^2 we can introduce the factorization

$$\widetilde{\Phi}_{\mathcal{F}}(\lambda) = \prod_{q=1}^{\widetilde{M}} \left(1 - \frac{\lambda^2}{\tilde{\lambda}_{2q}^2}\right), \tag{80}$$

which gives in real space

$$u(s) = \prod_{q=1}^{\widetilde{M}} \left[1 + \frac{D^2}{\tilde{\lambda}_{2q}^2}\right] \hat{u}(s). \tag{81}$$

Each of the doublets of the complex roots $(\tilde{\lambda}_{2q}, -\tilde{\lambda}_{2q})$ of $\widetilde{\Phi}_{\mathcal{F}}(\lambda)$ defines an internal length scale and the multiplicative structure of the operator (81) suggests that these scales generate a nested set of displacement fields $\tilde{u}_q(s)$ with $0 \leq q \leq \widetilde{M}$. The first and the last one represent the meso-scopic and the microscopic fields, respectively: $\tilde{u}_0 = \hat{u}$, $\tilde{u}_{\widetilde{M}} = u$. On the intermediate scales we can define the fields $\tilde{u}_q$ by the following set of recurrent differential relations

$$\tilde{u}_q(s) = \left[1 + \frac{D^2}{\tilde{\lambda}_{2q}^2}\right] \tilde{u}_{q-1}(s). \tag{82}$$

In this setting to move from smaller to larger scale one needs to perform a coarse-graining using an exponential kernel (inversion of the Helmholtz operator) carrying the corresponding averaging scale. The nested structure of the approximation is therefore explicit.

7 Case study: infinite domain

In this section we consider an adaptation of our additive multi-scale quasicontinuum model to the chain with first and second nearest neighbors interactions (NNN model). This is the simplest nontrivial case because the model with nearest neighbor interactions (NN model) is degenerate due to the absence of complex roots of the characteristic equation.

7.1 The discrete model

The only material parameters in the discrete NNN model are the elasticities of the NN and NNN bonds: Ψ_1 and Ψ_2. The characteristic equation reads

$$\Phi_{\mathcal{F}}(\lambda) = \frac{4}{a}\sin^2\left(\frac{a}{2}\lambda\right)\left[K - 4\Psi_2\sin^2\left(\frac{a}{2}\lambda\right)\right] = 0, \tag{83}$$

where $K = (\Psi_1 + 4\,\Psi_2)$ is the homogenized modulus (19). One can see that the roots of (83) depend on the moduli Ψ_1 and Ψ_2 through their ratio

$$\mu = \frac{\Psi_1}{4\Psi_2} \tag{84}$$

which is then the main non-dimensional parameter of the problem. Equation (83) has four complex roots in B. As we know, two of them coincide, forming the trivial double root $\lambda_0 = \lambda_1 = 0$. The other two roots necessarily appear in the form of a symmetric couple $(\lambda_2, \lambda_3 = -\lambda_2)$. Depending on the value of the parameter μ, there are three domains with different behavior. If $-1 \le \mu \le 0$, then the nontrivial roots are real and the infinite chain is unstable [12]. If $\mu \le -1$, these roots are purely imaginary

$$\lambda_2 = \frac{i}{a}\,\ln\left(2\sqrt{\mu(\mu+1)} - 2\mu - 1\right). \tag{85}$$

We can write $\lambda_2 = i/l_2$ and define an internal length scale

$$l_2 = \frac{a}{\ln\left[2\sqrt{\mu(\mu+1)} - (2\mu+1)\right]}. \tag{86}$$

If $\mu \ge 0$, we have two nontrivial roots on the boundary of the domain $\mathbb{B}$ forming a pseudo-quadruplet

$$\lambda_2 = \frac{\pi}{a} + \frac{i}{a}\,\ln\left(2\sqrt{\mu(\mu+1)} + 2\mu + 1\right). \tag{87}$$

In this case we can write $\lambda_2 = \pi/a + i/l_2$, which implies lattice scale binary oscillations modulated at scale l_2. For simplicity, we limit the subsequent analysis to a (generic) case $\mu \le -1$ (see [12] for more details on other cases).

Under the assumptions made, the discrete displacement field generated by the applied loads can be obtained from (12), where the Green's function is given by

$$G(n) = -\frac{|n|a}{2K} + \frac{l_2\,\mathrm{e}^{-|n|a/l_2}}{2K\kappa_2}. \tag{88}$$

Here we used the notation

$$\kappa_2 = \frac{l_2}{a}\,\sinh\left(\frac{a}{l_2}\right) = \frac{2\sqrt{\mu(\mu+1)}}{\ln\left(2\sqrt{\mu(\mu+1)} - 2\mu - 1\right)}. \tag{89}$$

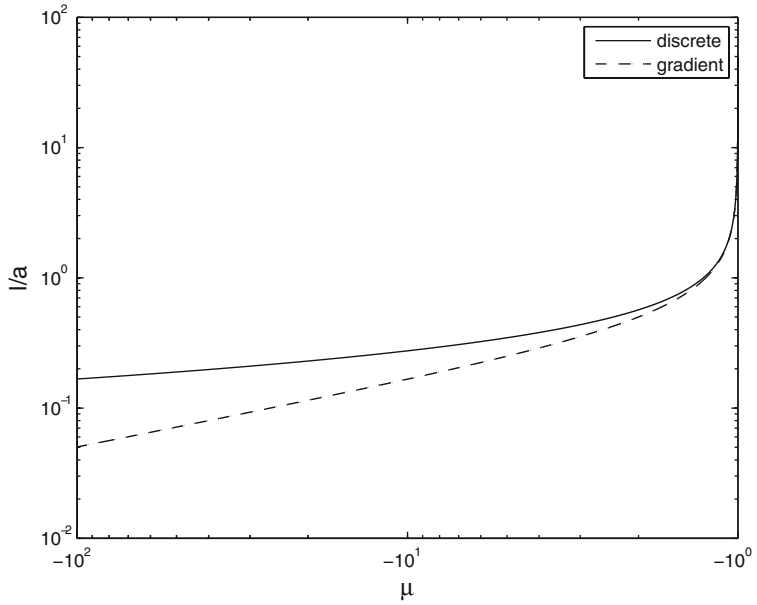

Fig. 1 The μ-dependence of the internal length scales in the discrete NNN model and in its gradient approximation: discrete $-l_2$, gradient $-l_2^*$. Notice the logarithmic scaling of the axes

7.2 Strain gradient elasticity

To obtain the strain gradient approximation of the NNN model we can use the general formula (36). We obtain

$$\Phi^*_{\mathcal{F}}(\lambda) = Ka\lambda^2\Big[1 - \frac{\lambda^2}{\lambda_2^{*2}}\Big], \tag{90}$$

where $\lambda_2^* = \pm i/l_2^*$ and

$$l_2^* = \frac{a}{2\sqrt{|\,\mu + 1\,|}}. \tag{91}$$

This length scale is different from the length parameter l_2 appearing in discrete theory (86). The two parameters are plotted as a function of μ in Fig. 1. One can see that the domain where l_2^* and l_2 are comparable, and where one can expect the gradient model to approximate the discrete model quantitatively, lies in the immediate vicinity of the point $\mu = -1$. As we have already mentioned, in this domain the homogenized modulus K softens and the internal length scale l_2 becomes macroscopic ($l_2 \gg a$).

7.3 Padé interpolation

We now follow (55) and write the truncated fractional decomposition for the Fourier image of the inverse elasticity operator

$$\big[\Phi^*_{\mathcal{F}}(\lambda)\big]^{-1} = \frac{1}{Ka\lambda^2} - \frac{1}{Ka\kappa_2}\left(\frac{1}{\lambda^2 - \lambda_2^2}\right). \tag{92}$$

The first term in the right hand side represents classical elasticity while the second term is responsible for boundary layers at scale l_2. In the physical space we obtain the following specialization of the integro-differential equation (59)

$$-K\left\{D^2u(s) + (1-\beta^2)\left[\frac{D^2u(s)}{\beta^2} - D\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-|s-\check{s}|/\beta l_2}}{2\beta l_2}\,Du(\check{s})d\check{s}\right]\right\} = f(s), \tag{93}$$

where $\beta = \sqrt{(\kappa_2 - 1)/\kappa_2}$. The elastic energy in the resulting nonlocal theory has the general form (61) where the nonlocal kernel $\mathcal{K}$ defined in (60) can now be written explicitly

$$\mathcal{K}(s) = K\,\delta(s) + \frac{K(1-\beta^2)}{\beta^2}\left[\delta(s) - \frac{\mathrm{e}^{-|s|/\beta l_2}}{2}\right]. \tag{94}$$

The expression for the nonlocal energy functional is

$$W(u) = \frac{K}{2}\int_{-\infty}^{\infty}\left\{\left[Du(s)\right]^2 + (1-\beta^2)\left[\left[\frac{Du(s)}{\beta}\right]^2 - \int_{-\infty}^{\infty} Du(s)\,\frac{\mathrm{e}^{-|s-\check{s}|/\beta l_2}}{2\beta l_2}\,Du(\check{s})d\check{s}\right]\right\} ds. \tag{95}$$

7.4 Multi-scale elasticity theory (additive)

In the context of the NNN model with $\mu < -1$ it is convenient to rewrite the generic decomposition (64) in the form

$$u(s) = u_c(s) + u_2^*(s) = u_c(s) + l_2\,v(s/l_2).$$

The associated microscopic energy is

$$W_2(v) = \frac{\kappa_2 K}{2}\int_{-\infty}^{\infty}\left\{\left[v'(s/l_2)\right]^2 + \left[v(s/l_2)\right]^2\right\} ds. \tag{96}$$

The general solution of the microscopic problem in the infinite domain with zero boundary conditions can be written as

$$v(s/l_2) = l_2^{-1}\int_{-\infty}^{\infty} G_2^*(s-\check{s})\,f(\check{s})\,d\check{s}. \tag{97}$$

Here

$$G_2^*(s) = -\frac{l_2\,\mathrm{e}^{-|s|/l_2}}{2K\kappa_2}.$$

is the Green's function of the "standard" microscopic problem.

7.5 Comparison of different approximations

The elasticity kernels for different approximations are compared with their discrete prototype in Fig. 2 where we consider a representative case of an NNN model with $\mu < -1$. One can see that despite the closeness of all approximations around $\lambda = 0$, the behavior of different models at short waves differers significantly. For instance, some theories are characterized by a bounded elasticity operator while others by an unbounded one. These deviations are irrelevant for the purposes of this paper since we limit our analysis to statics. However, they show that our theory can not be formally extended into dynamics by the addition of the macroscopic kinetic energy. The question of how the kinetic energy should be written will be addressed in a separate paper (see also [39]).

8 Case study: finite domain

In this Section we show how the generic forces applied at the exterior boundary of the chain generate "microscopic" boundary conditions in the additive multi-scale theory. For comparison we also derive the corresponding boundary conditions for the conventional strain-gradient elasticity.

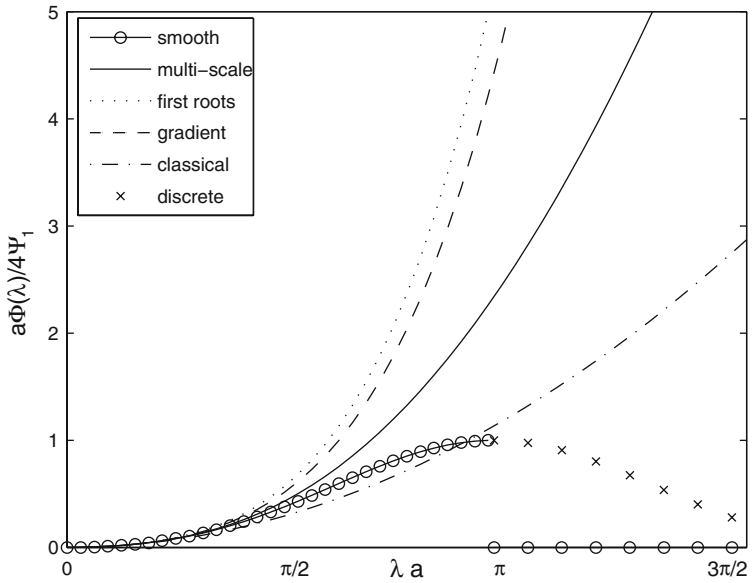

Fig. 2 Comparison of the elasticity kernels at real λ for different approximations of the NNN model with $\mu = -1.85$

8.1 The discrete model

The first step is to distinguish the microscopic and the macroscopic components of the loading. To emphasize ideas we again consider the simplest case of a one-dimensional NNN lattice.

Suppose that the chain is comprised of $(N+1)$ particles whose positions are given by the vector $(x_0, \dots, x_N)$. To highlight the inherent inhomogeneity of the reference configuration (due to external boundary layers), we shall continue working in this section with positions x_k instead of displacements u_k.

In these original variables the elastic energy of the chain can be written as

$$W = a\sum_{k=1}^{N}\left[\frac{\Psi_1}{2}\left(\frac{x_k - x_{k-1}}{a} - \xi_1\right)^2\right] + a\sum_{k=2}^{N}\left[\frac{\Psi_2}{2}\left(\frac{x_k - x_{k-2}}{a} - 2\,\xi_2\right)^2\right]. \tag{98}$$

We suppose that the chain is subjected to dead loading and write the work of external forces in the form

$$P = a\sum_{k=2}^{N-2} f_k\, x_k + F_N\, x_N + F_{N-1}\, x_{N-1} - F_0\, x_0 - F_1\, x_1. \tag{99}$$

Here we added to the bulk loading considered in the previous sections an additional four forces F_N, F_{N-1}, F_0, F_1 applied at the exterior boundaries of the chain. These forces are balanced in the sense that: $F_0 + F_1 - F_N - F_{N-1} = a\sum_{k=2}^{N-2} f_k$.

While the 'macroscopic' forces on the boundary F_c^- and F_c^+ can be defined unambiguously

$$F_c^- = F_0 + F_1, \quad F_c^+ = F_N + F_{N-1}, \tag{100}$$

the definition of the 'microscopic' forces requires some preparation and will be postponed till later in the paper (see also [12]).

An equilibrium displacement field x_k must satisfy the system of $(N+1)$ equations. They can be naturally split into the system of $(N-3)$ bulk equations (5)

$$\frac{\Psi_1}{a^2}\left(x_{k+1} + x_{k-1} - 2\,x_k\right) + \frac{\Psi_2}{a^2}\left(x_{k+2} + x_{k-2} - 2\,x_k\right) = -f_k, \tag{101}$$

with $2 \le k \le N-2$ and four additional boundary equations furnishing the boundary conditions for (101)

$$F_0 = \frac{\Psi_1}{a}(x_1 - x_0) + \frac{\Psi_2}{a}(x_2 - x_0) - \Psi_1 \xi_1 - 2\Psi_2 \xi_2 \tag{102}$$

$$F_1 = \frac{\Psi_1}{a}(x_2 + x_0 - 2x_1) + \frac{\Psi_2}{a}(x_3 - x_1) - 2\Psi_2 \xi_2 \tag{103}$$

$$F_{N-1} = -\frac{\Psi_1}{a}(x_N + x_{N-2} - 2x_{N-1}) + \frac{\Psi_2}{a}(x_{N-1} - x_{N-3}) - 2\Psi_2 \xi_2 \tag{104}$$

$$F_N = \frac{\Psi_1}{a}(x_N - x_{N-1}) + \frac{\Psi_2}{a}(x_N - x_{N-2}) - \Psi_1 \xi_1 - 2\Psi_2 \xi_2. \tag{105}$$

We proceed by solving the equilibrium problem in this general setting which gives us a benchmark to test various quasi-continuum approximations.

8.2 Solution of the discrete problem

To simplify comparison with the continuum case we introduce the total length of the chain $2L = Na$, and define a fictitious homogeneous reference lattice with atomic positions $s_k = k\,a - L$. The general solution of the homogeneous problem (101, 102) can be represented as a sum of two terms [12]

$$\bar{x}(s) = \bar{x}_c(s) + \bar{x}_{\rm m}(s) \tag{106}$$

The first term describes the homogeneous strain

$$\bar{x}_c(s) = \left[\frac{F_c^- + F_c^+}{2K} + \tilde{\varepsilon}\right] s \tag{107}$$

which depends on the macro-scopic forces F_c^- and F_c^+, homogenized modulus K and the classical prestress

$$\tilde{\varepsilon} = \frac{\Psi_1 \xi_1 + 4\Psi_2 \xi_2}{\Psi_1 + 4\Psi_2}. \tag{108}$$

The second term in (106) describes the fine structure of the boundary layers at the extremities of the chain

$$\bar{x}_{\rm m}(s) = -\frac{a}{\sinh\left(\frac{a}{l_2}\right)}\left\{\left[\frac{F_m^+}{K} + \check{\varepsilon}\right]\frac{\cosh\left(\frac{L+s}{l_2}\right)}{\sinh\left(\frac{2L}{l_2}\right)} - \left[\frac{F_m^-}{K} + \check{\varepsilon}\right]\frac{\cosh\left(\frac{L-s}{l_2}\right)}{\sinh\left(\frac{2L}{l_2}\right)}\right\}. \tag{109}$$

It depends on the micro-forces defined by

$$F_m^+ = F_N - (2\mu + 1)F_{N-1}, \quad F_m^- = F_0 - (2\mu + 1)F_1 \tag{110}$$

and the micro-level hyper-prestress [12]

$$\check{\varepsilon} = \frac{\Psi_1(\xi_1 - \xi_2)}{\Psi_1 + 4\Psi_2}. \tag{111}$$

A particular solutions of the inhomogeneous bulk equations can be written as

$$x_k = a\sum_{p=2}^{N-2} G(s_k, s_p) f_p, \tag{112}$$

where the Green's function can be split into the sum of two terms

$$G(s, \check{s}) = G_c(s - \check{s}) + G_{\rm m}(s, \check{s}). \tag{113}$$

The first term

$$G_{\rm c}(s-\check{s}) = -\frac{|s-\check{s}|}{2\,K} \tag{114}$$

represents the classical macroscopic contribution. The second term

$$G_{\rm m}(s,\check{s}) = -a\,\frac{\cosh\left(\frac{s+\check{s}}{l_2}\right)+\cosh\left(\frac{2L-|s-\check{s}|}{l_2}\right)}{2\,K\,\sinh\left(\frac{a}{l_2}\right)\,\sinh\left(\frac{2L}{l_2}\right)} \tag{115}$$

is responsible for the microscopic boundary layers of width l_2 around the points of application of the point forces.

We can now combine the solutions of the homogeneous and inhomogeneous problems. If we once again separate the classical macroscopic component of the displacement field $x_c(s_k)$ from its microscopic counterpart $x_{\rm m}(s_k)$, we obtain

$$x_k = x_c(s_k) + l_2\,w(s_k/l_2), \tag{116}$$

where

$$x_c(s) = \left[\frac{F_c^- + F_c^+}{2\,K} + \tilde{\varepsilon}\right] s + a\sum_{p=2}^{N-2} G_c(s-s_p)\,f_p, \tag{117}$$

and

$$w(s/l_2) = -\frac{a}{l_2\,\sinh\left(\frac{a}{l_2}\right)}\left\{\left[\frac{F_m^+}{K}+\check{\varepsilon}\right]\frac{\cosh\left(\frac{L+s}{l_2}\right)}{\sinh\left(\frac{2L}{l_2}\right)} - \left[\frac{F_m^-}{K}+\check{\varepsilon}\right]\frac{\cosh\left(\frac{L-s}{l_2}\right)}{\sinh\left(\frac{2L}{l_2}\right)}\right\} + \frac{a}{l_2}\sum_{p=2}^{N-2} G_{\rm m}(s,s_p)\,f_p. \tag{118}$$

It is not hard to see that one can recover from (118) the general formulas from Sect. 2 for the infinite domain when $L/a \to \infty$ and $l_2 \sim a$.

8.3 Classical elasticity

In the classical continuum approximation the elastic energy for the NNN model takes the form

$$W_{\rm c} = \frac{K}{2}\int_{-L}^{+L}\left[x_c'(s)-\tilde{\epsilon}\right]^2 ds. \tag{119}$$

The work of the macro forces can be written as

$$P_{\rm c} = F_c^+\,x_c(L) - F_c^-\,x_c(-L) + \int_{-L}^{+L} f(s)\,x_c(s)\,ds, \tag{120}$$

where we introduced the continuum distribution of bulk forces

$$f(s) \equiv \sum_{k=2}^{N-2} f_k\,\delta\Big(\frac{s-s_k}{a}\Big). \tag{121}$$

To find the coarse field $x_c(s)$ we need to solve the standard equation of elastostatics

$$K\,x_c''(s) = -f(s), \text{ for } -L < s < L, \tag{122a}$$

supplemented by the classical boundary conditions

$$K\left[x_c'(s)-\tilde{\varepsilon}\right]=F_c^{\pm},\ \text{at}\ s=\pm L. \tag{122b}$$

The system (122) can be solved explicitly and we obtain

$$x_c(s)=\Big[\frac{F_c^+ + F_c^-}{2\,K}\ +\ \tilde{\varepsilon}\Big]s\ +\ \int\limits_{-L}^{L} G_c(s-\check{s})\,f(\check{s})d\check{s}. \tag{123}$$

One can see that the function $x_c(s)$ delivers an exact interpolation of the discrete macro-solution $x_k=x_c(s_k)$ (see (117)).

8.4 Strain gradient model

Assume now that the internal length scale a, while being much smaller than the external length scale L, is not zero. We can then go beyond the classical elasticity and, following the recipes from Sect. 4.2 and 7.2, construct a strain-gradient approximation. The remaining task is to supplement the equilibrium equations (38) with the boundary conditions implied by the discrete theory.

Instead of simply borrowing the formulas from the analysis of the problem in the infinite domain, it is instructive to re-derive the bulk equations together with the boundary conditions without using the Fourier transform. The details of the preliminary asymptotic reduction of the total energy are presented in the Appendix C (see also [8]). To simplify the expression for the energy further we need to recall our conclusion in Sect. 4.2 that the strain-gradient theory is not very helpful unless the characteristic length scale l_2^* is much larger than a. In the interval of interest, $\mu\ \leq\ -1$, this happens when $\mu\ \sim\ -1$ (see Fig. 1). More precisely, gradient approximation is expected to work only in the range where $K\ll|\Psi_p|$ for $p=1,2$, which is equivalent to the condition $|1+\mu|\ll\ 1$. In what follows we assume the following natural scaling

$$|1+\mu|\sim\Big(\frac{a}{l_2^*}\Big)^2, \tag{124}$$

which allows us to further simplify the expression for the energy given in Appendix C.

It will be convenient to split the total energy into the bulk and surface parts. For the bulk elastic energy we obtain

$$W_b=\frac{K}{2}\int\limits_{-L}^{+L}\Big[\big(x'(s)-\tilde{\epsilon}\big)^2-\frac{\Psi_2\,a^2}{K}\,x''^2(s)\Big]\,ds. \tag{125}$$

The corresponding potential energy reads

$$P_b=\int\limits_{-L}^{+L} f(s)\,x(s)\,ds. \tag{126}$$

The surface term in the energy can be written as

$$W_s=-a\,\Psi_2\sum_{s=\pm L}\big(x'(s)-\xi_2\big)\big[x'(s)-\xi_2-\ a\,n(s)\,x''(s)\big] \tag{127}$$

where $n(\pm L)=\pm 1$. The potential energy of surface loading is then

$$P_s=F_c^+\,x(L)\ -\ F_c^-\,x(-L)-a\,F_{N-1}\Big[x'(L)-\frac{a}{2}\,x''(L)\Big]\ -\ a\,F_1\Big[x'(-L)+\frac{a}{2}\,x''(-L)\Big]. \tag{128}$$

An implicit assumption behind our asymptotic development is that the macroscopic forces are scaled with the bulk modulus K. Then, since we are in the softening regime with $K\sim(a/l_2^*)^2$, the zero order term does

not exist and the lowest order term in the total energy is associated with the surface (see also [8]). It can be written as

$$W_1 - P_1 = -\Psi_2 \sum_{s=\pm L} \Big[x'(s) - \xi_2\Big]^2 + F_{N-1}\, x'(L) \;+\; F_1\, x'(-L). \tag{129}$$

By minimizing this functional we obtain the following boundary conditions

$$x'(-L) = \frac{F_1}{2\Psi_2} + \xi_2, \quad x'(L) = \frac{F_{N-1}}{2\Psi_2} + \xi_2. \tag{130}$$

In the next order in a/l_2^* one has to minimize the following functional

$$W_2 - P_2 = \int_{-L}^{+L} \left\{ \frac{K}{2}\Big[x'(s) - \tilde{\epsilon}\Big]^2 - \frac{\Psi_2\, a^2}{2}\, x''^2(s) - f(s)\, x(s) \right\} ds - \; F_c^+\, x(L) + F_c^-\, x(-L) \tag{131}$$

with the kinematically imposed boundary conditions (130). The corresponding Euler–Lagrange equations take the form

$$\Psi_2\, a^2 x''''(s) + K\, x''(s) = -f(s), \text{ for } -L < s < L. \tag{132}$$

The two additional boundary conditions, derived from the variational principle (131), are

$$\Psi_2\, a^2 x'''(s) + K\, x'(s) = F_c^{\pm} + \Psi_1 \xi_1 + 4\Psi_2 \xi_2, \text{ for } s = \pm L. \tag{133}$$

The linear equations (132) supplemented by the boundary conditions (130) and (133)) can be solved explicitly. The solution $x(s)$ can be represented as a sum of the coarse-grained field $x_c(s)$ and a micro-scopic correction of the boundary layer type

$$x(s) = x_c(s) + l_2^* w^*(s/l_2^*). \tag{134}$$

The classical field $x_c(s)$ is already known (see (117). The micro-field $w^*(s/l_2^*)$ can also be given in the closed form

$$\begin{aligned} w^*\left(\frac{s}{l_2^*}\right) = &-\left[\frac{F_m^+}{K} + \check{\varepsilon}\right] \frac{\cosh\left(\frac{L+s}{l_2^*}\right)}{\sinh\left(\frac{2L}{l_2^*}\right)} + \left[\frac{F_m^-}{K} + \check{\varepsilon}\right] \frac{\cosh\left(\frac{L-s}{l_2^*}\right)}{\sinh\left(\frac{2L}{l_2^*}\right)} \\ &- \int_{-L}^{L} \left[\frac{\cosh(\frac{s+\check{s}}{l^*}) + \cosh\left(\frac{2L-|s-\check{s}|}{l_2^*}\right)}{2\, K\, \sinh\left(\frac{2L}{l_2^*}\right)}\right] f(\check{s})\, d\check{s}. \end{aligned} \tag{135}$$

Observe that the function w^* in (135) could also be obtained from the analogous discrete solution w in (118) by substituting the parameter l_2 with l_2^* and replacing the factor κ_2 by 1. Therefore the agreement between the strain gradient and discrete theories improves as $\mu \to -1$ because then $l_2 \to l_2^*$ and $\kappa_2 \to 1$. As we move away from this domain of parameters, characterized by the "soft" response of the homogenized macro theory, the discrete solution begins to vary at scale a and the gradient approximation becomes exceedingly poor.

8.5 Multi-scale continuum theory (additive)

To capture the lattice effects in the broader range of parameters we shall now follow the algorithm of the additive multi-scale elasticity theory developed in Sect. 6. For the NNN model with $\mu < -1$ our algorithm produces the same additive decomposition of the displacement field as in the discrete theory

$$x(s) = x_c(s) + l_2\, w(s/l_2).$$

The first term in this ansatz satisfies equations of macroscopic elasticity and is explicitly given by (117). The energy of the microscopic field reads

$$W_{\rm m} = \frac{\kappa_2\, K}{2} \int_{-L}^{+L} \left\{ w^2(s/l_2) + \left[w'(s/l_2) + \frac{\check{\varepsilon}}{\kappa_2} \right]^2 \right\} ds. \tag{136}$$

The microscopic potential energy can be written as

$$P_{\rm m} = -l_2 \int_{-L}^{L} f(s)\, w(s/l_2)\, ds - l_2 \Big[F_m^+\, w(L/l_2) - F_m^-\, w(-L/l_2) \Big]. \tag{137}$$

Here the macro-micro interaction (or rather reaction) term (integral term in (137)) provides the crucial coupling between the coarse grained classical description and the fine scale description at the level of the lattice.

It is straightforward to show that the continuum multi-scale model with the total energy $W_{\rm m} - P_{\rm m}$ generates the desired interpolation of the generic discrete solution. In fact, we need to check only the microscopic boundary layer contribution. The Euler-Lagrange equation for the function w takes the form

$$\frac{K\,\kappa_2}{l_2} \left[w''(s/l_2) - w(s/l_2) \right] = f(s). \tag{138a}$$

The corresponding boundary conditions are

$$K \left[\kappa_2\, w'(s/l_2) + \check{\varepsilon} \right] = -F_m^{\pm}, \ \text{for } s = \pm L. \tag{138b}$$

The microscopic field can be obtained as the general solution of the homogeneous problem (138) plus a particular solution of the inhomogeneous problem. We omit the details of the derivation and write directly the final formula

$$w(s/l) = \left[-\left\{ \frac{F_m(\check{s}) + F_c(\check{s})}{K} - \check{\varepsilon} \right\} \frac{\cosh\left(\frac{s+\check{s}}{l_2}\right)}{\kappa_2\, \sinh\left(\frac{2L}{l_2}\right)} \right]_{\check{s}=-L}^{\check{s}=L} - \int_{-L}^{L} \left[\frac{\cosh(\frac{s+\check{s}}{l_2}) + \cosh\left(\frac{2L\, -|s-\check{s}|}{l_2}\right)}{2\, K\, \kappa_2\, \sinh\left(\frac{2L}{l_2}\right)} \right] f(\check{s})\, d\check{s} \tag{139}$$

One can see that this continuum solution indeed represents an exact interpolation of the discrete solution (118).

While the macro-problem (122) is completely independent of the micro-problem (138) and can be solved directly as soon as the macroscopic loading is known, the micro-problem is not fully independent of the macro-problem due to the presence of the "reaction" macro-forces. As we have already seen in the general case, the macro-forces in the micro-problem can be eliminated under the assumption that the macro-solution is known. The problem at the micro-level, which then uses the coarse solution as the source term, takes the form

$$\frac{\kappa_2}{l_2} \left[w''(s/l_2) - w(s/l_2) \right] = -x_c''(s), \tag{140a}$$

$$\kappa_2\, w'(-L/l_2) = \frac{2(\mu+1)F_1}{K} + \xi_2 - x_c'(-L), \tag{140b}$$

$$\kappa_2\, w'(L/l_2) = \frac{2(\mu+1)F_{N-1}}{K} + \xi_2 - x_c'(L). \tag{140c}$$

This linear problem can be again solved explicitly

$$w(s/l_2) = \left[\frac{F_{N-1}}{2\,\Psi_2} + \xi_2 \right] \frac{\cosh\left(\frac{L+s}{l_2}\right)}{\kappa_2\, \sinh\left(\frac{2L}{l_2}\right)} - \left[\frac{F_1}{2\,\Psi_2} + \xi_2 \right] \frac{\cosh\left(\frac{L-s}{l_2}\right)}{\kappa_2\, \sinh\left(\frac{2L}{l_2}\right)} - \frac{x_c(s)}{\kappa_2\, l_2} + \int_{-L}^{L} \widetilde{G}(s,\check{s}) \frac{x_c(\check{s})}{\kappa_2\, l_2^2}\, d\check{s}. \tag{141}$$

The finite domain Green's function, which "feels" the boundaries of the body, is of the form

$$\widetilde{G}(s,\check{s}) = \frac{\cosh(s+\check{s}) + \cosh\left(\frac{2L}{l_2} - |s-\check{s}|\right)}{2\,\sinh\left(\frac{2L}{l_2}\right)}. \tag{142}$$

The total displacement field $x(s)$ can now be expressed in terms of the macro-field $x_c(s)$ as

$$x(s) = l_2\left[\frac{F_{N-1}}{2\,\Psi_2} + \xi_2\right]\frac{\cosh\left(\frac{L+s}{l_2}\right)}{\kappa_2\,\sinh\left(\frac{2L}{l_2}\right)} - l_2\left[\frac{F_1}{2\,\Psi_2} + \xi_2\right]\frac{\cosh\left(\frac{L-s}{l_2}\right)}{\kappa_2\,\sinh\left(\frac{2L}{l_2}\right)}$$
$$+ \frac{\kappa_2 - 1}{\kappa_2}\,x_c(s) + \int_{-L}^{L} \widetilde{G}(s,\check{s})\frac{x_c(\check{s})}{\kappa_2\,l_2}\,d\check{s}. \tag{143}$$

In the particular case when the domain is infinite and all fields decay sufficiently fast, this nonlocal relation can be rewritten in a simpler form

$$x(s) = \frac{\kappa_2 - 1}{\kappa_2}\,x_c(s) + \int_{-\infty}^{\infty} \exp\left(-\frac{|\check{s}-s|}{l_2}\right)\frac{x_c(\check{s})}{2\,\kappa_2\,l_2}\,d\check{s}. \tag{144}$$

The formula (144) can be also obtained directly from (72) by double integration by parts.

9 Conclusions

In this paper we propose a multi-scale quasicontinuum theory aimed at reproducing the fine structure of the linear elastic lattice fields. The new theory uses the minimal amount of information about the discrete elasticity operator to interpolate the solution of the discrete problem exactly. The interpolating continuum theory is usually perceived to be necessarily nonlocal. We show that the local representation of such theory is possible if one considers several displacement fields: a coarse macro-scopic field and micro-scopic corrections, describing the internal and external boundary layers at particular micro-scales. The relevant micro-scales are dictated by the discrete theory, depend in a nontrivial way on the ratios of micro-scopic elastic moduli and may deviate considerably from the lattice parameter. The main advantage of the new model is that it allows one to reduce the system of finite difference equations or an equivalent integral equation emerging in strongly nonlocal continuum theory to a series of local problems requiring solution of a sequence of partial differential equations of the second order. The overall dimensionality of the corresponding approximation problem depends on the chosen cut off distance.

Because of its use of the "natural" microscopic fields, the new theory has some similarity with the classical models of Timoshenko in the theory of beams and of Reissner–Mindlin in the theory of plates. It can also be linked to some recent phenomenological theories introducing various nonlocal measures of damage in softening materials (e.g. [24,32,33]).

The basic structure of the new theory can be also analyzed from the perspective of the so-called *explicit* and *implicit* theories of elastic continua with microstructure aiming at the improvement upon the classical homogenized limit. In this interpretation, if the operator of the microscopic theory is $\Phi_{\mathcal{F}}(\lambda)$ and the classical macroscopic limit is $\Phi^c_{\mathcal{F}}(\lambda)$, the explicit approach (e.g. [4,23]) would be to look for approximation in the form $\Phi^*_{\mathcal{F}}(\lambda) \sim \Phi^c_{\mathcal{F}}(\lambda)(1+Q)$, where $Q \sim \lambda^2 + \cdots$ is a polynomial in λ. On the contrary, the implicit approach (e.g. [4,5]) is based on the expansion $\Phi^*_{\mathcal{F}}(\lambda) \sim \Phi^c_{\mathcal{F}}(\lambda)(1/(1+P))$, where $P \sim -\lambda^2 + \cdots$ is also a polynomial. In these terms, our additive model leads to the expansions of the form $\Phi^{*-1}_{\mathcal{F}}(\lambda) \sim \Phi^{c-1}_{\mathcal{F}}(\lambda) + 1/Q_1 + 1/Q_2 + \cdots$, where Q_i are some standard second order polynomials. The last expression can also be rewritten as $\Phi^*_{\mathcal{F}}(\lambda) \sim \Phi^c_{\mathcal{F}}(\lambda)(1 + S/R)$, where S and R are polynomials. One can see that the new theory can be viewed as a synthesis of explicit and implicit approximation schemes. The main difference of our approach from its mostly phenomenological predecessors is the transparent link to the underlying lattice model allowing one to replace the guesses concerning the structure of the polynomials Q and P, by the specific computations generating the polynomials S and R.

In conclusion we mention that despite its ability to match an exact benchmark test, the new model is still heuristic and needs to be supplemented by the rigorous theorems clarifying the degree of closeness of the approximate continuum solutions to their discrete counterparts. The corresponding technical questions are expected to be surmountable. Also, in this paper the model is intentionally presented in its simplest version which deals with a linear scalar field in one dimension. Again, the generalization to vector fields and to multiple dimensions and even to linear elastodynamics appear to be straightforward. The real challenge is posed by the extension of the ideas of this paper to the nonlinear case and by the development of applications in such fields as dislocation theory and fracture mechanics.

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Appendix A

Here we briefly consider a chain with NNNN interactions (see also [38]), whose elastic energy can be written in the form

$$W(x) = a \sum_{k\in\mathbb{Z}} \sum_{p=1}^{3} \frac{\Psi_p}{2} \left[\frac{x_{k+p} - x_k}{a} - p\,\xi_p \right]^2 .$$

The Fourier-transform of the elastic operator is

$$\Phi_{\mathcal{F}}(\lambda) = \frac{4}{a} \sin^2\left(\frac{a}{2}\lambda\right)\Big[K - 4(\Psi_2 + 6\Psi_3)\sin^2\left(\frac{a}{2}\lambda\right) + 16\Psi_3 \sin^4\left(\frac{a}{2}\lambda\right)\Big]. \tag{145}$$

where the homogenized modulus is

$$K = \frac{1}{2a}\,\Phi''_{\mathcal{F}}(0) = \Psi_1 + 4\,\Psi_2 + 9\,\Psi_3.$$

The necessary and sufficient conditions for stability of such NNNN chains can be stated as the conditions of the positive definiteness of the right hand side of (145) at real λ inside the Brillouin zone. We obtain two domains of stability

$$\left\{K \geq \Psi_3 \left(\frac{\Psi_2}{2\Psi_3} + 3\right)^2 > 0\right\} \quad \text{and} \quad \Big\{K \geq 2\Big[|\Psi_2 + 2\Psi_3| + \Psi_2 + 2\Psi_3\Big]\Big\}.$$

In the stable domains the characteristic equation has the following structure of the roots (in $\mathbb{B}$): two trivial roots at $\lambda = 0$ and either four nontrivial roots forming a quadruplet or two couples of roots with either $\Re e(\lambda) = 0$ or $\Re e(\lambda) = \pm\pi/a$. The (generic) case of four purely imaginary roots, which generates two different internal length scales, is the simplest. If we define $\mu_p = \Psi_p/\Psi_3$ for $p = 1, 2$ we can explicitly formulate the corresponding restrictions on the elastic moduli in the form

$$-(\mu_2 + 2) \pm \sqrt{\mu_2^2 - 4(\mu_1 + \mu_2)} \;\geq\; 4,$$

$$\mu_1 + 4\mu_2 + 9 \geq 0,\ \ \mu_2 \leq -6,\ \text{ and } \quad \mu_1 + 1 \leq \left(\frac{\mu_2}{2} - 1\right)^2 .$$

When these conditions are satisfied, the desired purely imaginary roots are $\lambda_{2,4} = (i/a)\ln(\rho_{2,4})$, where

$$\rho_{2,4} = \frac{-(\mu_2 + 2) \pm \sqrt{\mu_2^2 - 4(\mu_1 + \mu_2)} + \sqrt{\left[-(\mu_2 + 2) \pm \sqrt{\mu_2^2 - 4(\mu_1 + \mu_2)}\right]^2 - 16}}{4}.$$

Appendix B

Here we consider in more detail the microscopic theory for the field $u^{**}_m(s) = [u^*_m(s) + \overline{u^*_m}(s)]/2$ in the case when the corresponding roots of the characteristic equation form a symmetric quadruplet. In this case the pair of related terms in (55) can be rearranged as a single term $\left[(\Phi^{**}_m)_{\mathcal{F}}(\lambda)\right]^{-1}$, where

$$(\Phi_m^{**})_{\mathcal{F}}(\lambda) = \left[\frac{\lambda_{2m}}{\Phi'_{\mathcal{F}}(\lambda_{2m})(\lambda^2-\lambda_{2m}^2)} + \frac{\bar{\lambda}_{2m}}{\Phi'_{\mathcal{F}}(\bar{\lambda}_{2m})(\lambda^2-\bar{\lambda}_{2m}^2)}\right]^{-1}$$
$$= A\big(\lambda^2 + |\lambda_{2m}|^2\gamma_m^2\big) - B$$
$$+\left[\frac{A|\lambda_{2m}|^4\gamma_m^4 - B|\lambda_{2m}|^2\gamma_m^2 + C}{2|\lambda_{2m}|\gamma_m}\right]\left[\frac{1}{\lambda-|\lambda_{2m}|\gamma_m} - \frac{1}{\lambda+|\lambda_{2m}|\gamma_m}\right]$$

and

$$A = \frac{|\Phi'_{\mathcal{F}}(\lambda_{2m})|^2}{2\Re e\big(\lambda_{2m}\Phi'_{\mathcal{F}}(\bar{\lambda}_{2m})\big)},\ B = 2A\Re e\big(\lambda_{2m}^2\big),\ C = A|\lambda_{2m}|^4,\ \text{and}\ \gamma_m^2 = \frac{\Re e\big(\lambda_{2m}\Phi'_{\mathcal{F}}(\lambda_{2m})\big)}{\Re e\big(\lambda_{2m}\Phi'_{\mathcal{F}}(\bar{\lambda}_{2m})\big)}.$$

By making an inverse Fourier transform we obtain

$$\Phi_m^{**}(s) \equiv \Big[-AD^2 + A|\lambda_{2m}|^2\gamma_m^2 - B\Big]\delta(s) + \frac{A|\lambda_{2m}|^4\gamma_m^4 - B|\lambda_{2m}|^2\gamma_m^2 + C}{2|\lambda_{2m}\gamma_m|}\,\mathrm{e}^{i|\gamma_m\lambda_{2m}s|}$$

if $\gamma_m^2 < 0$, or

$$\Phi_m^{**}(s) \equiv \Big[-AD^2 + A|\lambda_{2m}|^2\gamma_m^2 - B\Big]\delta(s) + \frac{A|\lambda_{2m}|^4\gamma_m^4 - B|\lambda_{2m}|^2\gamma_m^2 + C}{2|\lambda_{2m}|\gamma_m}\,\sin\big(\gamma_m|\lambda_{2m}s|\big)$$

if $\gamma_m^2 > 0$. In the physical space we obtain the following integral equation

$$\int_{-\infty}^{\infty} \Phi_m^{**}(s-\check{s})u_m^{**}(\check{s})\,d\check{s} = f(s).$$

The solution of this equation can be written in the form

$$u_m^{**}(s) = \int_{-\infty}^{\infty} G_m^{**}(s-\check{s})f(\check{s})\,d\check{s} \equiv a\sum_{p\in\mathbb{Z}} G_m^{**}(s-pa)f_p$$

where

$$G_m^{**}(s-\check{s}) = \frac{1}{2}\left[\frac{i\,\mathrm{e}^{i\lambda_{2m}|s|}}{\Phi'_{\mathcal{F}}(\lambda_{2m})} + \frac{i\,\mathrm{e}^{-i\bar{\lambda}_{2m}|s|}}{\Phi'_{\mathcal{F}}(-\bar{\lambda}_{2m})}\right]. \tag{146}$$

Notice that in this case the "canonical" micro-problem is strongly nonlocal. The comparison of the kernel G_m^{**} in (146) with the kernel $\hat{G}_m$ in (21) shows that we obtained an exact interpolation of the corresponding discrete field.

Appendix C

We begin by rewriting (98) in the form where the attribution of the energy to particular lattice points is explicit

$$W = \frac{\Psi_1}{4a}\left\{(x_1-x_0)^2 + (x_N-x_{N-1})^2 + \sum_{k=1}^{N-1}\big[(x_k-x_{k-1})^2 + (x_{k+1}-x_k)^2\big]\right\}$$
$$+\frac{\Psi_2}{8a}\left\{(x_2-x_0)^2 + (x_N-x_{N-2})^2 + \sum_{k=1}^{N-1}\big[(x_k-x_{k-2})^2 + (x_{k+2}-x_k)^2\big]\right\}$$

$$+\frac{\Psi_2}{8a}\left\{(x_1-x_{-1})^2+(x_{N+1}-x_{N-1})^2+2\sum_{k=1}^{N-1}(x_{k+1}-x_{k-1})^2\right\}$$
$$-\frac{\Psi_2}{4a}\left[(x_1-x_{-1})^2+(x_{N+1}-x_{N-1})^2\right]-(\Psi_1\xi_1+2\Psi_2\xi_2)(x_N-x_o)$$
$$-2\Psi_2\,\xi_2\,(x_{N-1}-x_1)\;+\;L\left(\Psi_1\,\xi_1^2\right)\;+\;(2L-a)\left(2\Psi_2\,\xi_2^2\right).$$

Here we used the assumption that the energy of the bonds is equipartitioned between the associated lattice points. Next we assume that the approximating continuum field $x(s)$ is sufficiently smooth and that one can define a characteristic length scale $l^*\sim x'(s)/x''(s)$. We further assume that the non-dimensional parameter a/l^* is small and that we can expand the displacement field in Taylor series with respect to this parameter (see [8] for more formal analysis). If we substitute such expansion into the energy and drop terms of the order higher than $(a/l^*)^3$ we obtain

$$W-P=a\left\{\left(\frac{\Psi_1+4\Psi_2}{4}\right)\sum_{s=\pm L}x'^2(s)+\sum_{k=1}^{N-1}\left(\frac{\Psi_1+4\Psi_2}{2}\right)x'^2(s_k)\right\}$$
$$+a^2\left\{\sum_{s=\pm L}\left[\left(\frac{\Psi_1}{16}+\frac{\Psi_2}{2}\right)x''^2(s)+\left(\frac{\Psi_1+4\Psi_2}{12}+\frac{\Psi_2}{2}\right)x'(s)\,x'''(s)\right]\right.$$
$$\left.+\sum_{k=1}^{N-1}\left[\left(\frac{\Psi_1}{8}+\Psi_2\right)x''^2(s_k)+\left(\frac{\Psi_1+4\Psi_2}{6}+\Psi_2\right)x'(s_k)\,x'''(s_k)\right]\right\}$$
$$-\sum_{s=\pm L}\left\{(\Psi_1\xi_1+4\Psi_2\xi_2)\,n(s)\,x(s)+a\left[\Psi_2\left(x'(s)-\xi_2\right)^2\right]\right.$$
$$\left.+a^2\left[\left(\frac{\Psi_1}{4}+\Psi_2\right)x'(s)\;+\Psi_2\,\xi_2\right]n(s)\,x''(s)+\frac{\Psi_2\,a^3}{3}\left(x'(s)-\xi_2\right)x'''(s)\right\}$$
$$+2L\left(\frac{\Psi_1}{2}\,\xi_1^2+2\Psi_2\,\xi_2^2\right)\;-(F_N+F_{N-1})\,x(L)+(F_0+F_1)\,x(-L)$$
$$-a\sum_{k=2}^{N-2}f(s_k)\,x(s_k)\;+a\,F_{N-1}\left[x'(L)-\frac{a}{2}\,x''(L)\right]+a\,F_1\left[x'(-L)+\frac{a}{2}\,x''(-L)\right]$$

Here, as in the main text, we used the notation $n(\pm L)=\pm 1$. To switch from sums to integrals we can use the trapezoidal quadrature formula and then after integrating by parts we obtain

$$W-P=\int_{-L}^{+L}\left\{\left(\frac{\Psi_1+4\Psi_2}{2}\right)\left[x'(s)-\frac{\Psi_1\xi_1+4\Psi_2\xi_2}{\Psi+4\Psi_2}\right]^2\right.$$
$$\left.-\frac{a^2}{2}\left(\Psi_2+\frac{\Psi+4\Psi_2}{12}\right)x''^2(s)-f(s)\,x(s)\right\}ds$$
$$-a\sum_{s=\pm L}\left\{\Psi_2\left(x'(s)-\xi_2\right)^2-\;a\left[\Psi_2\left(x'(s)-\xi_2\right)\;-\left(\frac{\Psi_1+4\Psi_2}{6}\right)x'(s)\right]n(s)\,x''(s)\right\}$$
$$-(F_N+F_{N-1})\,x(L)\;+\;(F_0+F_{N-1})\,x(-L)$$
$$+a\,F_{N-1}\left[x'(L)-\frac{a}{2}\,x''(L)\right]\;+\;a\,F_1\left[x'(-L)+\frac{a}{2}\,x''(-L)\right].$$

We use this expression as the starting point in Sect. (8.4)

References

1. Aifantis, E.C.: Higher order gradients and size effects. In: Carpinteri, A. (Ed.) Size-scale effects in the failure mechanisms of materials and structures, pp. 231–242. Ed. F.N. Spon, London (1996)

2. Arndt, M., Griebel, M.: Derivation of higher order gradient continuum models from atomistic models for crystalline solids. Multiscale Model. Simul **4**, 531–562 (2005)
3. Askes, H., Suiker, A.S.J., Sluys, L.J.: A classification of higher-order strain-gradient models—linear analysis. Arch. Appl. Mech. **72**, 171–188 (2002)
4. Askes, H., Sluys, L.J.: Explicit and implicit gradient series in damage mechanics. E. Journ. Mec. A/Solids **21**, 379–390 (2002)
5. Askes, H., Gutierrez, M.: Implicit gradient elasticity. Int. J. Numer. Methods Eng. **67**, 400–416 (2006)
6. Bardenhagen, S., Triantafyllidis, N.: Derivation of higher order gradient continuum theories in 2,3-D nonlinear elasticity from periodic lattice models. J. Mech. Phys. Solids **42**, 111–139 (1994)
7. Berezhnyy, M., Berlyand, L.: Continuum limit for three-dimensional mass-spring networks and discrete Korn's inequality. J. Mech. Phys. Solids **54**, 635–669 (2006)
8. Blanc, X., Le Bris, C., Lions, P.-L.: From molecular models to continuum mechanics. Arch. Rational. Mech. Anal **164**, 341–381 (2002)
9. Born, M., Huang, K.: Dynamical Theory of Crystal Lattices. Oxford University Press, Oxford (1954)
10. Braides, A., Gelli, K.: From Discrete to Continuum: A variational approach. Lecture Notes SISSA, Trieste (2000)
11. Braides, A., Truskinovsy, L.: Asymptotic expansions by Γ convergence. Cont. Mech. Trermodyn **20**, 21–62 (2008)
12. Charlotte, M., Truskinovsky, L.: Linear chain with a hyper-pre-stress. J. Mech. Phys. Solids **50**, 217–251 (2002)
13. Collins, M.A.: A quasi-continuum approximation for solitons in an atomic chain. Chem. Phys. Lett **77**, 342–347 (1981)
14. Dobson, M., Elliot, R.S., Luskin, M., Tadmor, E.B.: A multilattice quasicontinuum for phase transforming materials: cascading Cauchy–Born kinematics. J. Comput. Aided Mater. Des. **14**, 219–237 (2007)
15. DiVincenzo, D.P.: Dispersive corrections to continuum elastic theory in cubic crystals. Phys. Rev. B **34**, 5450–5465 (1986)
16. W.E., Huang, Z.: A dynamic atomistic continuum method for the simulation of crystalline materials. J. Comput. Phys. **182**, 234–261 (2002)
17. Weinan, E., Lu, J., Yang, J.: Uniform accuracy of the quasicontinuum method. Phys. Rev. B **74**, 214115 (2006)
18. Kevrekidis, P.G., Kevrekidis, I.G., Bishop, A.R., Titi, E.S.: Continuum approach to discreteness. Phys. Rev. E **65**, 046613 (2002)
19. Koiter, W.T.: Couple stresses in the theory of elasticity, I and II. Proc. K. Ned. Acad. Wet. (B) **67**, 17–44 (1964)
20. Krantz, S.G.: Handbook of Complex Variables. Birkhäuser, Boston (1999)
21. Krumshansl: Generalized continuum field representation for lattice vibrations. In: Wallis, R.F. (ed.) Lattice Dynamics, pp. 627–634. Pergamon, London (1965)
22. Kunin, I.: Elastic Media With Microstructure, v.I (One dimensional models). Springer, Berlin (1982)
23. Lazar, M., Maugin, G., Aifantis, E.: Dislocations in second gradient elasticity. Int. J. Solids Struct. **43**, 1787–1817 (2006)
24. Lorentz, E., Andrieux, S.: Analysis of nonlocal models through energetic formulations. Int. J. Solids Struct. **40**, 2905–2936 (2003)
25. Lin, P.: Convergence analysis of a quasi-continuum approximation for a two-dimensional material without defects. SIAM J. Numer. Anal. **45**, 313–332 (2007)
26. Maranganti, R., Sharma, P.: A novel atomistic appoach to determine strain-gradient elasticity constants. J. Mech. Phys. Solids **55**, 1823–1852 (2007)
27. Martinsson, P.G., Babuska, I.: Mechanics of materials with periodic truss or frame micro-structures. Arch. Rational. Mech. Anal. **185**, 201–234 (2007)
28. Mechanics of generalized continua. In: Kroener, E. (ed.) Proc. IUTAM-Symposium. Springer, Berlin (1968)
29. Miller, R.E., Tadmor, E.B.: The quasi-continuum method:overview, applications and current directions. J. Comput. Aided Mater. Des. **9**, 203–239 (2002)
30. Mindlin, R.: Second gradient of strain and surface tension in linear elaticity. Int. J. Solids Struct. **1**, 417–438 (1965)
31. Ortiz, M., Philips, R., Tadmor, E.B.: Quasicontinuum analysis of defects in solids. Phil. Mag. A **73**, 1529–1563 (1996)
32. Peerlings, R.H.J., Geers, M.G.D., de Borst, R., Brekelmans, W.A.M.: A critical comparison of non-local and gradient enhanced softening continua. Int. J. Solids Struct. **38**, 7723–7746 (2001)
33. Polizzotto, C.: Unified thermodynamic framework for nonlocal/gradient continuum theories. European J. Mech. A/Solids **22**, 651–668 (2003)
34. Rogula, D.: Nonlocal Theory of Elastic Media. Springer, Berlin (1982)
35. Silling, S.A.: Reformulation of elasticity theory for discontinuities and long-range forces. J. Mech. Phys. Solids **48**, 175–209 (2000)
36. Sunyk, R., Steinmann, P.: On higher gradients in continuum-atomistic modelling. Int. J. Solids Struct. **40**, 6877–6896 (2003)
37. Toupin, R.A.: Elastic materials with couple stresses. Arch. Rational. Mech. Anal **11**, 385–414 (1962)
38. Truskinovsky, L., Vainchtein, A.: Quasicontinuum modelling of short wave instabilities in crystal lattices. Phil. Mag. **85**, 4055–4065 (2005)
39. Truskinovsky, L., Vainchtein, A.: Quasicontinuum models of dynamic phase transitions. Continuum. Mech. Thermodyn. **18**, 1–21 (2006)