



Nonlocal constitutive laws generated by matrix functions: Lattice dynamics models and their continuum limits

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ABSTRACT

We analyze one-dimensional discrete and quasi-continuous linear chains of $N \gg 1$ equidistant and identical mass points with periodic boundary conditions and generalized nonlocal interparticle interactions in the harmonic approximation. We introduce elastic potentials which define by Hamilton's principle discrete "Laplacian operators" ("Laplacian matrices") which are operator functions ($N \times N$ -matrix functions) of the Laplacian of the Born–von-Karman linear chain with next neighbor interactions. The non-locality of the constitutive law of the present model is a natural consequence of the *non-diagonality* of these Laplacian matrix functions in the N dimensional vector space of particle displacement fields where the periodic boundary conditions (cyclic boundary conditions) and as a consequence the (Bloch-)eigenvectors of the linear chain are maintained. In the quasi-continuum limit (long-wave limit) the Laplacian matrices yield "Laplacian convolution kernels" (and the related elastic modulus kernels) of the non-local constitutive law. The elastic stability is guaranteed by the positiveness of the elastic potentials. We establish criteria for "weak" and "strong" nonlocality of the constitutive behavior which can be controlled by scaling behavior of material constants in the continuum limit when the interparticle spacing $h \rightarrow 0$. The approach provides a general method to generate physically admissible (elastically stable) *non-local constitutive laws* by means of "simple" Laplacian matrix functions. The model can be generalized to model non-locality in $n = 2, 3, \dots$ dimensions of the physical space.

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1. Introduction

There is a wide range of materials and deformable structures at nanoscale for which local constitutive descriptions appear to be inappropriate. For instance material systems such as carbon nanotubes show on the nanoscale size effects which strongly suggest the importance of non-local inter-particle interactions and as a consequence the non-locality of the constitutive laws which cannot be covered by classical local continuum theories. The importance of non-local constitutive behavior was raised by several authors already in the sixties of the last century such as Eringen (1972, 1983, 1992, 2002), Kröner (1967), Krumhansl (1968) and Kunin (1982). Born–von-Karman models and their continuum counterparts account

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only for local inter-particle interactions represented by next- or close neighbor particle springs (Askar, 1985; Born & Huang, 1954; Eringen & Kim, 1977; Maradudin, Montroll, & Weiss, 1963; Scriver, 1990; Truskinovsky & Vainchtein, 2005) and as a consequence these models predict dispersion free wave propagation in the continuum limit (long-wave limit). Hence these classical models are only able to describe the effects of local inter-particle interactions on the vibrational properties. In order to account for size effects in elastic nano-structures, theoretical models with nonlocal interactions were raised recently for beams, plates and shells (Challamel & Wang (2008), Lu, Zhang, Lee, Wang, & Reddy (2007), Lim (2010), Reddy (2007) and references therein).

Over the three last decades, there has been an explosion of interest and activity on the dynamics of nonlinear waves in lattices. In these works, the weak non-localities are induced by the atomic interactions between first, second and close neighbor particles which are generally modeled by nonlinear springs (see for e.g.: Askar (1982), Cadet (1987), Collet (1993), Maugin (1999), Pouget (2005) and Remoissenet & Flytzanis (1984)) The quasi-continuum approximation is used, which permits to show that lattice dynamics can be approximatively described by nonlinear partial differential equations of Bousinesq or Korteweg–de Vries and nonlinear Schrödinger type which admit solutions of soliton type (kink, breather, asymmetric envelope or dark solitons) modulating a carrier wave whose wave vector is not limited by the continuum limit approximation. In the same context, an interesting approach concerns the so-called continualization method applied to dynamics of dense chains and lattices was presented by Rosenau (2003).

Despite those advanced linear and nonlinear models there is further need of analytical models to cover aspects of non-locality and interconnecting both the lattice dynamics approach and the continuum approach. To this end the goal of the present paper is to introduce simple non-local periodic 1D lattice (linear chain) models which lead to non-local behavior in the discrete linear chain, and to deduce the corresponding non-local constitutive law in the continuum limit. We show in the present paper that scaling relations of the material constants in the continuum limit are required in order to guarantee that the elastic energy remains finite. The starting point for our models are positive elastic energies which define by Hamilton's variational principle generalized Laplacian operators with all required "good properties" of Laplacians including elastic stability.

So far there is a huge lack of non-local constitutive models in the literature accounting for the interlink between lattice dynamics and continuum approach. In most classical works on non-locality such as of Eringen (1983, 2002), Lazar, Maugin, and Aifantis (2006), Maugin (1979, 1999) and others such as Kröner (1967), Kunin (1982) and Eringen (1972, 1983, 1992) non-locality is phenomenologically introduced for some constitutive convolution kernels of simple forms or by inclusion of some "convenient" higher order gradient type models such as by Eringen (2002), Lazar et al. (2006) and Maugin (1979). However, most of those models are pure continuum models and were not linked to lattice dynamics models.

A three-dimensional lattice model was introduced by Eringen and Kim (1977) which analyzed the link between lattice dynamics and non-local elasticity in three dimensions by considering the continuum limit of small interparticle distance for non-local harmonic springs to describe harmonic far-range interactions. Nevertheless, there seems to be still a lack of more general approaches which deduce non-local constitutive continuum models rigorously from discrete lattice dynamics models. The present paper aims to contribute in this respect by introducing non-locality by a discrete (linear chain) lattice approach and by analyzing its continuum limit. The starting point are harmonic elastic potentials defined on a periodic linear chain which include non-local harmonic interparticle interactions and define by Hamilton's variational principle discrete non-local constitutive laws of matrix forms which take in the continuum limit non-local convolutional forms.

The paper is organized as follows: We introduce a one-dimensional linear chain model with non-local harmonic interactions and periodic boundary conditions. We generate the non-local constitutive behavior by constructing elastic potentials which lead via Hamilton's variational principle to "Laplacian operators" which are operator functions (matrix functions in the N -dimensional space of particle displacements) of the local "Laplacian" of the next-neighbor Born–von Karman linear chain model. In a sense we conceive the "local Laplacian" operator as "generator" of "non-local Laplacian" operators.

We analyze the vibrational dispersion relation (negative eigenvalues of the Laplacian) of the discrete chain with periodic boundary conditions and analyze its continuum limit (long-wave limit) rigorously. The Laplacian then takes in the long-wave limit the form of the non-local convolutional constitutive law which contains also the full information on the elastic modulus kernel. The "degree of nonlocality" of these kernels is sensitive on the scaling behavior of the material constants in the continuum limit.

2. Discrete non-local model for the 1D linear chain quasi-continuous and its continuum limits

We consider a linear chain of N identical particles where $N \gg 1$ is assumed to be "large" and $u_p = u(x_p)$ denotes a field variable such as the displacement field associated to particle p located at lattice points $x_p = ph$ ($p = 0, \dots, N - 1$). We assume equidistant particles with interparticle spacing h (lattice constant) and identical particle masses μ . The length of the linear chain is indicated by $L = Nh$. We use a compact notation by means of distributions and functional calculus. We assume the periodic boundary conditions (cyclically closed chains)

$$u(x_p) = u(x_{p+N}). \quad (1)$$

Due to the periodicity of the boundary conditions we use throughout this paper particle indices p cyclically, such that $0 \leq p \leq N - 1$ (When we generate matrix functions with indices $p \notin \{0, 1, \dots, N - 1\}$ outside this set, the cyclic index

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