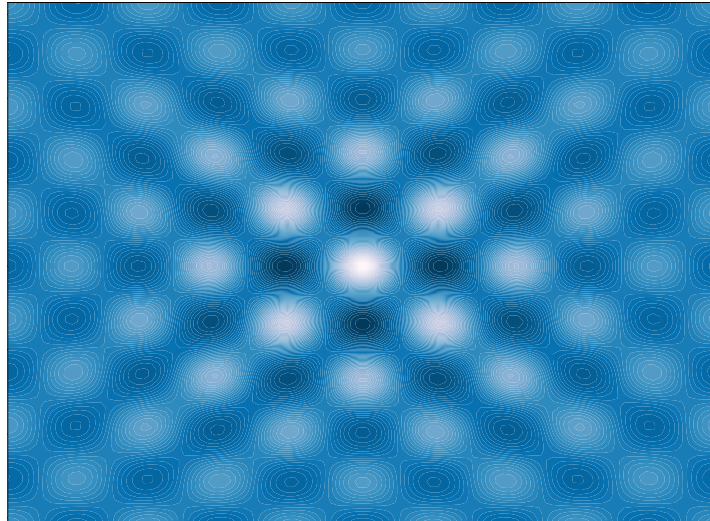




Curriculum 3. Modelling and Simulation

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Nonlocal discrete systems with mass preserving springs Dynamics and design criteria for metamaterials



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Abstract

The dynamics of periodic structures and lattices are gaining increasing attention in engineering and physics in wave manipulation devices across various scales and applications. In mechanics, nonlocal configurations incorporating beyond-nearest-neighbour (BNN) couplings are especially promising, as they can show “roton-like” dispersion relations at a macroscale, thus phase and group velocities with opposite signs and backwards wave propagation. While it is true that BNN connections offer novel possibilities in designing new architected and meta-materials, existing models and prototypes seem to lack criteria for comparing local and nonlocal lattices or a sound framework for transitioning between these configurations. A key issue arises from the usage of monoatomic mass-spring models as theoretical paradigms for analysing their dynamics, where usually the mass of atoms is considered for the inertia of the system, while the mass of the springs is neglected. However, as the number of nonlocal pairings increases, the mass of the springs grows, potentially reaching a magnitude competing with the oscillating masses, thus leading to possible model inconsistencies. To fill this gap, in the first part of this PhD thesis a physically reasonable principle that monoatomic one-dimensional chains must obey to pass from single- to multi-connected systems is proposed through a mass conservation law for elastic springs, thereby introducing a suitable real dimensionless parameter α to tune stiffness spatial distribution over the system domain. Therefore, the dispersion relations as a function of α and of the degree of nonlocality P are derived analytically, demonstrating that the proposed principle can be rather interpreted as a general mechanical consistency condition to preserve proper dynamics, fixing the spring to atom mass ratio. The analyses are carried out through analytical and numerical investigations on discrete nonlocal lattices, both finite and infinite, imposing Bloch-Floquet periodicity conditions. Numerical dispersion relations are obtained through two-dimensional Fast Fourier Transforms, which highlight the applicability of the proposed principle to finite nonlocal chains, for which boundary effects are also discussed. The second part of the thesis focuses on applications of the proposed principle to models which presents a slightly nonlinear behaviour, due to a nonlinear elastic restoring force. The relationship between nonlocality and nonlinearity in a one-dimensional monoatomic chain is investigated. The conservation law is then generalized and enforced for nonlinear couplings, so the level of nonlocality P and the stiffness distribution parameter α are still used to govern the dynamics of the nonlinear nonlocal chains. The results obtained are employed to yield perturbed and nonlinear amplitude-dependent dispersion relations for nonlocal, mass-preserving monoatomic chains. In the third part of the thesis, the presence of defects is taken into account. In fact, another major leap forward in metamaterial design in the last decade was the discovery of the impact of crystal symmetries on the topological properties of materials. These properties are often based on defects or irregularities in the lattice symmetries, which can be usefully employed to obtain waveguides and localization phenomena. Finally, the last part concerns the application of the proposed modelling strategy to two-dimensional lattices, taking into consideration in-plane and out-of-plane displacements in the dynamic behaviour of flat structures. The conservation law with its tuning parameters α and P is expanded and applied to two-dimensional Bravais lattices. At the end, dispersion curves are retrieved for nonlocal two-dimensional lattices and the results are discussed, envisioning opportunities for conceiving new classes of nonlocal metamaterials.

Publications

Guarracino F., Fraldi M., and Pugno N.M.. “Local-to-Non-Local Transition Laws for Stiffness-Tuneable Monoatomic Chains Preserving Springs Mass”. In: Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences 382.2279 (Sept. 23, 2024), p. 20240037. issn: 1364-503X, 1471-2962. doi: 10.1098/rsta.2024.0037, (Chapter 2)

Guarracino F., Fraldi M., N.M. Pugno, “Mass conservation criteria for nonlocal stiffness-tuneable weakly nonlinear monoatomic chains”, proceedings of the XXVI AIMETA congress, 2024, under review, (Chapter 4)

Manuscripts in preparation

Guarracino F., Fraldi M., N.M. Pugno, “Dynamic analysis of mass-conserving weakly nonlinear non-local discrete systems”, in preparation, (Chapter 3)

Guarracino F., Fraldi M., N.M. Pugno, “Localisation phenomena in a mass-conserving beyond nearest neighbour coupled monoatomic chain”, in preparation, (Chapter 4)

Guarracino F., Fraldi M., N.M. Pugno, “Mass conservation criteria for bidimensional Bravais lattices with nonlocal couplings”, in preparation, (Chapter 5).

Contents

Chapter 1

Introduction: wave propagation in periodic structures

1.1 Phononic crystals

Phononic crystals are periodic, artificially engineered materials, which are specifically designed to manipulate elastic and acoustic waves and alter their propagation properties ([1], [2]). The name *phononic* is derived from *phonons*, i.e. the quanta of vibrational energy in crystals, studied in solid state physics. In the realm of electromagnetic wave propagation, their counterparts are *photonic* crystals, introduced in the mid 60s as light manipulation devices [3].

Materials in which waves propagate can be fluids, in liquid or gas form, or solid. Acoustic waves propagate in fluids, while elastic waves propagate in solids. Even though they have a common ground from a physical point of view, their mathematical treatment differs. Acoustic waves can be described as pressure waves, which can be described by a time-dependent scalar field in three-dimensional space. On the other hand, elastic waves are described by a vector field of particle displacements. Moreover, elastic waves support polarization and they can propagate in an anisotropic fashion in solids, even in natural crystals.

The term phononic crystal usually refers to a device for pressure wave manipulation, but the term can also be used for elastic waves in literature. In order to build a phononic crystal for pressure waves, artificial crystals include periodic layering or inclusions of different fluids, as gas inclusions in a liquid. Artificial crystals for elastic wave propagation, instead, are composed by a homogeneous or heterogeneous structure of solid elements.

Crystals, natural or artificial, are composed by periodically repeated unit cells, made of one or multiple materials. One of the main differences between natural and artificial crystals lies in the size of the so-called *lattice constant*, i.e. the distance separating two unit cells of the periodic structure. The macroscale of the lattice constants in phononic crystals allows them to be studied through classical mechanics and wave propagation in solids.

Typically, crystals are classified by the number of periodicities they present: one-dimensional (1D), two-dimensional (2D) or three-dimensional (3D).

The wave propagation directions depend on the waves involved, for instance sonic waves exhibit one mode of propagation, while elastic waves can polarise in three different modes. Therefore a difference is usually made between *sonic* and phononic crystals, where the first involve the propagation of pressure waves, as in fluids.

They can be employed in different areas, ranging from microwaves to acoustic, from ultrasonic to audible waves. The phononic crystals peculiarity is the presence of a bandgap, that is, a frequency interval in which wave propagation is inhibited. Bandgaps can be defined as partial or complete, respectively if they involve only one or more directions of propagation. The presence of band gaps

allows for the design of mirrors, cavities and guides for elastic and acoustic waves. Another peculiar property of these crystals is their *dispersive* behaviour, which corresponds to a nonlinear relation between frequencies and wavenumbers.

Among popular engineering applications, the following can be considered:

- Vibration isolation, as metamaterials and phononic crystals can be employed to reduce the vibrations in several environments, for instance in transportation or industry;
- Noise damping, as phononic crystals can be employed in compact acoustic shields, with a wide reach to low frequency isolation thanks to local resonances;
- Waveguides, in order to control and steer the energy propagation direction, also for surface waves;
- Energy harvesting through resonant cavities;
- Sensors, through actuators, generators and transducers;
- Acoustic and elastic wave lenses, in order to focus them or to achieve exotic phenomena as negative refraction and reflection;
- Components for Micro-electro-mechanical (MEMS) devices.

and many others which require wave interactions and manipulation.

1.1.1 Notes on wave propagation in elastic solids

The content of this thesis focuses on propagation of scalar waves in discrete periodic media, therefore it will not consider polarization, anisotropy and so on. As defined in [4], by considering functions of the type $x(t, x_1, x_2, x_3)$, the equation describing wave propagation in three-dimensions is the following:

$$\frac{\partial^2 x}{\partial t^2} = c^2 \nabla^2 x \quad (1.1)$$

while if the spatial coordinate is only one, e.g. x the equation reduces to:

$$\frac{\partial^2 x}{\partial t^2} = c^2 \frac{\partial^2 x}{\partial x_1^2} \quad (1.2)$$

where c is the celerity and has the units of a velocity, m/s. For a rod, in which the motion causes a change in the axial length as deformation, the stress takes the form

$$\sigma = \frac{E \Delta L}{L} \quad (1.3)$$

where E is the Young's modulus of the material, and

$$c^2 = \frac{E}{\rho} \quad (1.4)$$

with ρ material density.

The general solution reads

$$x = g(x_1 - ct) + G(x_1 + ct) \quad (1.5)$$

where g and G are arbitrary functions depending on the initial conditions, with g corresponding to a plane wave travelling along the positive direction of the x -axis and G to the one propagating in the

opposite direction. For each wave it can be noticed that the deformation of the elastic medium has a certain shape at time t and at time $t + \Delta t$ the same shape will be found at a distance $c(\Delta t)$ along the x axis. In an isotropic medium the velocity of plane waves propagating parallel to the x, y, z axes is c in any direction. Moreover, the constant c^2 does not depend on the position for homogeneous media.

For instance, if the coordinates belong to $x \in [0, L]$, the left end of the element could be vibrating with a sinusoidal function

$$x(0, t) = \Omega \sin(\omega t) \quad (1.6)$$

where Ω is the amplitude of the excitation and $\omega = 2\pi f$ is the angular frequency and $f = 1/T$ the frequency in Hertz and T the period. After a time Δt has passed, the wavefront will be found in a position x along the axis. The displacement of this point is described by

$$x(x_1, t) = \Omega \sin(\omega t - \kappa x_{1,eq}) \quad (1.7)$$

where $x_{1,eq}$ is the initial position, κx is a phase factor, given by the position times a quantity named wavenumber, given by

$$\kappa = \frac{\omega}{c}. \quad (1.8)$$

1.1.2 Bragg scattering

Periodic lattices enable wave manipulation through two main mechanisms: Bragg scattering and local resonances. Thanks to these mechanisms, they are able to create the so called *band gaps*, which are frequency ranges where wave propagation is forbidden. In fact, the transmission of waves in periodic systems follows the general boundary problem where incident waves will be transmitted or reflected. If the frequency encountered by the lattice is part of those inside a stop band or a band gap in the dispersion relation, then the coefficient of reflection will be $R = 1$ and no waves will be transmitted.

Bragg scattering is one of the phenomena phononic lattices are built on. It constitutes a condition for interference of waves scattered by the periodic structure. When the wavelength of a wave is comparable to the spacing between the elements in the lattice, constructive or destructive interference patterns emerge. Specifically, when the condition $\Delta x_1 = \lambda/2$ is met, where Δx_1 is the distance between scattering elements imagined in one dimension and λ is the wavelength, destructive interference occurs, preventing wave propagation. Therefore, band gaps where waves of certain frequencies cannot propagate through the structure appear. It is important to notice that this condition is tied to the characteristic size of the periodic structure, also called lattice constant a .

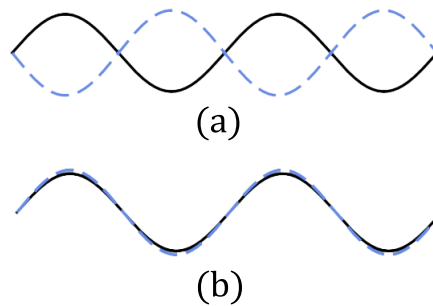


Figure 1.1: Destructive (a) and constructive interference (b), Adapted from <https://cmt-go.phys.ethz.ch/education/autumn-semester-2016-mechanical-metamaterials.html>.

1.1.3 Local resonances

Local resonance is another property that can have an effect on wave propagation in periodic structures. It relies on the presence of resonant elements within each unit cell of the lattice. The coupling causes the frequency spectrum to split and a band-gap to appear. Unlike Bragg scattering, the resonance frequency is determined by the properties of the coupled oscillators and not by the size of the structure. In fact, the strength of the coupling between the local resonator and the propagating wave affects the size of the band gap. This allows for the creation of band gaps at frequencies where the wavelength is much larger than the lattice constant.

In order to obtain a locally resonant system, two coupled oscillators have to be considered, $x(t)$ and $y(t)$, described by the following general equations of motion, with two oscillators with the same natural frequency:

$$\begin{aligned}\ddot{x}(t) &= -\omega_0^2 x(t) + \gamma y(t) \\ \ddot{y}(t) &= -\omega_0^2 y(t) + \gamma x(t)\end{aligned}\tag{1.9}$$

where ω_0 is the natural frequency of uncoupled oscillators and γ is the force of the coupling. The solutions of this equation system yield the eigenfrequencies of the coupled system. If the oscillators have different natural frequencies, ω_x and ω_y , the splitting effect will decrease, as the effect of coupling is greatest when the natural frequencies of the oscillators are close together.

1.1.4 Mathematical treatment of periodic lattices

Periodic materials are mathematically described by an unit cell that repeats itself over one, two or three dimensions, following the lattice basis vectors in the multiple directionality cases. Once the physical and geometrical features of the unit cell are fixed, the lattice is thus easily described. Figure 1.2 shows examples of this procedure, through which the periodic lattice is generated, adapted from [5].

Generally speaking, a periodic lattice of discrete particles can be generated from a number of base vectors corresponding to the number of dimensions of the lattice. If a three-dimensional lattice is considered, the lattice vectors are $\mathbf{a}_1, \mathbf{a}_2$ and $\mathbf{a}_3$. A point in the lattice can be individuated by

$$\mathbf{r} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3\tag{1.10}$$

with n_1, n_2, n_3 integers.

A two-dimensional lattice will be instead generated by two basis vectors $\mathbf{a}_1, \mathbf{a}_2$ and a one-dimensional lattice will develop along one axis.

The periodic lattices can hold different shapes based on the symmetries they present. From the study of crystal symmetries in solid state physics ([6], [7]), it is known that there is a limited number of different configurations that can be attained for every space dimension, named Bravais lattices. In one dimension there is only one configuration, defined by a series of points equally spaced along a line.

In two dimensions, five different Bravais lattices can be enumerated, namely:

- Oblique, which is the most general configuration as it is invariant only for rotations of 180° and 360° with respect to any point in the lattice;
- Rectangular, in which the base vectors are perpendicular to each other but have different length;
- Rhombic, similar to the rectangular lattice but with an additional element at the center of the rectangle;
- Hexagonal, with 120° angles between the base vectors;

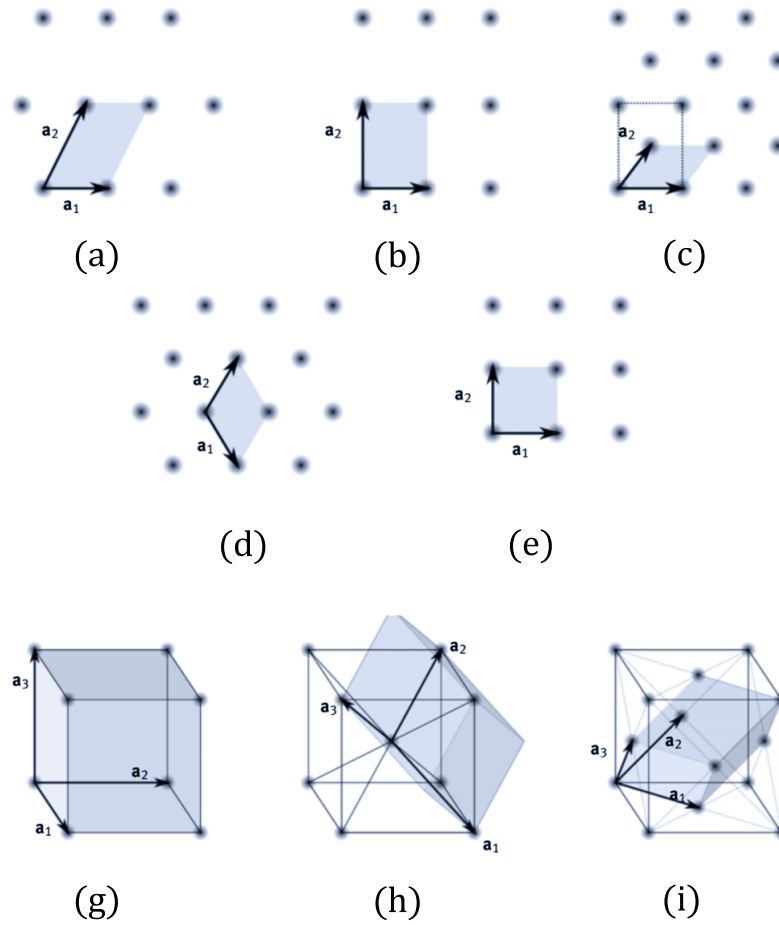


Figure 1.2: Bravais lattices in two and three dimensions, adapted from Laude [5]. The two dimensional Bravais lattices are (a) oblique, (b) rectangular, (c) rhombic, (d) hexagonal and (f) square. Three-dimensional cells are (g) simple cubic (SC), (h) body-centered cubic (BCC) and face-centered cubic (FCC).

- Square, with perpendicular base vectors that have the same length.

In three dimensions instead, the possible Bravais lattices amount to 14, divided in 7 systems based to the axial relations that describe the cells, namely:

- Triclinic, without any symmetries;
- Monoclinic, with one couple of perpendicular base vectors;
- Orthorhombic, where every base vector is perpendicular to the others;
- Tetragonal, as the orthorhombic but with two sides of equal length;
- Cubic, where all the base vectors are perpendicular and have the same length. It includes the simple cubic (SC), the body centered cubic (BCC) and the face centered cubic (FCC);
- Trigonal;
- Hexagonal.

Every point in the lattice is considered to be an element, i.e. a bead or an atom, having a mass m . This element is connected to one or more neighbouring elements through elastic connections, i.e. springs. Every particle in the lattice consequently acts as an harmonic oscillator, attracted to an equilibrium position by an elastic restoring force. If the elastic restoring force is different for the x, y, z directions, it will be an anisotropic oscillator, while if it is the same it will be an isotropic one. An isotropic harmonic oscillator is characterised by a proper frequency f_0 which only depends on the mass m of the particle and on the restoring force, while an anisotropic one by $f_{0,x}, f_{0,y}, f_{0,z}$ frequencies corresponding to the vibrations in the three directions.

In a one-dimensional lattice, an infinite row of isotropic harmonic oscillators is considered, with a spacing a from one another. This system will present an infinite number of resonance frequencies, or vibration modes, as the number of particles considered. The first mode is taken with infinite wavelength, which corresponds to a wavenumber $\kappa = 0$. This leads all of the particles to be displaced simultaneously and thus to the distance a between them not changing. The elastic restoring force does not come into play therefore the particles are not displaced from one another. However, when the frequency shifts, a relative displacement between the particles will take place in the vibration mode, up until a maximum frequency f_{max} , above which no other frequencies can propagate along the system.

This is represented by the dispersion relation in Figure 1.3 below, where the maximum frequency is also known as cut-off frequency.

In 1.1.1, a continuous, homogeneous and isotropic medium was taken into account. When considering the real axis x , the displacement of a point with respect to another was obtained through a translation operator $T_{\Delta x} = e^{i\kappa\Delta x}$, as

$$x(x_1, t) = e^{i(\kappa x_{eq} - \omega t)} \implies x(x_1 + \Delta x_{eq}, t) = e^{i\kappa\Delta x_{eq}} x(x_1, t) \quad (1.11)$$

When considering the discrete lattices described above, the displacement field $u_n(t)$ is defined over the integers numbers $n \in \mathbb{Z}$. Each element is located at $x = na$, with a lattice constant. On the other hand, the function $u(x, t)$ has values in $\mathbb{R}$ or $\mathbb{C}$. The plane wave solution can be expressed in the discrete lattice as

$$x_n(t) = e^{i(\kappa na - \omega t)} \quad (1.12)$$

the translation operator is then defined as $T_{n+1} = e^{i\kappa a}$, and

$$x_{n+1}(t) = e^{i\kappa a} e^{i(\kappa na - \omega t)} \quad (1.13)$$

This stems from the *Bloch theorem*, which enunciates that *the eigenmodes of the periodic Helmholtz equation are Bloch waves of the form*

$$x(\mathbf{r}) = e^{-i\boldsymbol{\kappa} \cdot \mathbf{r}} \tilde{x}(\mathbf{r}) \quad (1.14)$$

where $\tilde{x}(\mathbf{r})$ is a periodic function with the same periodicity of the lattice and $\boldsymbol{\kappa}$ is the Bloch wavevector.

When referring to wave propagation in periodic media, frequency domain analyses provide a helpful tool to retrieve the dynamic behaviour. Periodic Bloch-Floquet conditions are applied to the boundaries, and the sole unit cell is considered to be sufficient to analytically predict the overall chain behaviour.

1.1.4.1 Reciprocal space and Brillouin zones

The travelling wave solution in equation 1.13 is a periodic solution, as the values corresponding to $\kappa na = 2\pi$ are equal to those yielded by $\kappa na = 0$. The values are repeated with a periodicity

$\kappa = \kappa + 2\pi s$, with $s \in \mathbb{Z}$. This is why in the case of periodic lattices, the study refers to the *Brillouin zones*, which are the minimum areas to be considered in the *reciprocal lattice* to fully represent the lattice's dynamical behaviour.

The reciprocal lattice is defined as the lattice in which the Fourier transform of the wavefield of the direct lattice is represented. The reciprocal lattice is a Bravais lattice as well, and its Fourier transform yields the direct lattice. It is mathematically defined as

$$e^{-i(\boldsymbol{\kappa} \cdot \mathbf{r})} = 1 \quad (1.15)$$

In the one-dimensional case the first Brillouin zone in the reciprocal lattice corresponds to the following wavenumbers

$$\kappa \in \left[-\frac{\pi}{a}, \frac{\pi}{a} \right] \quad (1.16)$$

taking a value smaller or larger of κ would lead to retrieving the same solution in a previous or subsequent repetition. From 1.16, it can be noticed that the first Brillouin zone is defined by the lattice constant a , i.e. the value of its unit spacing.

Two- and three-dimensional direct lattices are defined as in equation 1.10. The reciprocal lattices' base vectors are defined as

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij} \begin{cases} i = 1, 2, 3 \\ j = 1, 2, 3 \end{cases} \quad (1.17)$$

with δ_{ij} Kronecker delta, which is defined as $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ otherwise. Thus the base vectors are orthogonal for $i \neq j$ and their lengths are $|\mathbf{b}_i| = 2\pi/|\mathbf{a}_j|$.

This means that the wavenumber space is now defined as, for instance in a three-dimensional lattice

$$\boldsymbol{\kappa} = h_1 \mathbf{b}_1 + h_2 \mathbf{b}_2 + h_3 \mathbf{b}_3 \quad (1.18)$$

with a 2π periodicity in every direction.

The concept of reciprocal space and Brillouin zones is important for understanding wave propagation in periodic structures. The reciprocal lattice is related to the periodicity of the real-space lattice, and the Brillouin zone defines the range of wave vectors $\boldsymbol{\kappa}$ that are physically distinct.

The scalar waves propagating into a multi-dimensional lattice can be expressed as:

$$\psi = e^{i(\omega t - \boldsymbol{\kappa} \cdot \mathbf{r})}, \quad (1.19)$$

where the phase is constant along the directions perpendicular to $\boldsymbol{\kappa}$, with $\boldsymbol{\kappa} \cdot \mathbf{r}_\perp = 0$.

From equations 1.10 and 1.18, the product $\boldsymbol{\kappa} \cdot \mathbf{r}$ can be expanded, and applying the orthogonality condition from equation 1.17 it simplifies to

$$\boldsymbol{\kappa} \cdot \mathbf{r} = 2\pi(h_1 n_1 + h_2 n_2 + h_3 n_3). \quad (1.20)$$

where the constants n_i, h_j are integers, so the resulting number from the sum and products in the brackets is also an integer. Therefore the definition in equation 1.15 is valid and

$$e^{i2\pi(h_1 n_1 + h_2 n_2 + h_3 n_3)} = 1 \quad (1.21)$$

from the reciprocal lattice definition.

1.1.5 Dispersion relations

Once the underlying mathematical concepts necessary for describing discrete lattices have been presented, it is possible to obtain the dynamical behaviour of said infinite periodic lattices. As anticipated, the displacements of any particle are attainable by writing the equations of motion of the unit cell. Considering a monoatomic chain with only nearest neighbour connections. All the masses and the springs are assumed to be identical, thus from Newton's second law:

$$m\ddot{x}_n(t) = k[x_{n-1} + x_{n+1} - 2x_n] \quad (1.22)$$

with m mass of the particle and k springs' stiffness.

By substituting the travelling wave solution from equation 1.12, the frequency domain representation of the chain is obtained as

$$-m\omega^2 e^{i(\kappa na - \omega t)} = k e^{i(\kappa na - \omega t)} (e^{-i(\kappa na)} + e^{i(\kappa na)} - 2) \quad (1.23)$$

from which the dispersion relation, remembering from Euler's formula that $\cos(\kappa na) = ((e^{-i(\kappa na)} + e^{i(\kappa na)})/2)$, can be retrieved as

$$\omega = \sqrt{\frac{2k}{m}(\cos(\kappa na) - 1)} \quad (1.24)$$

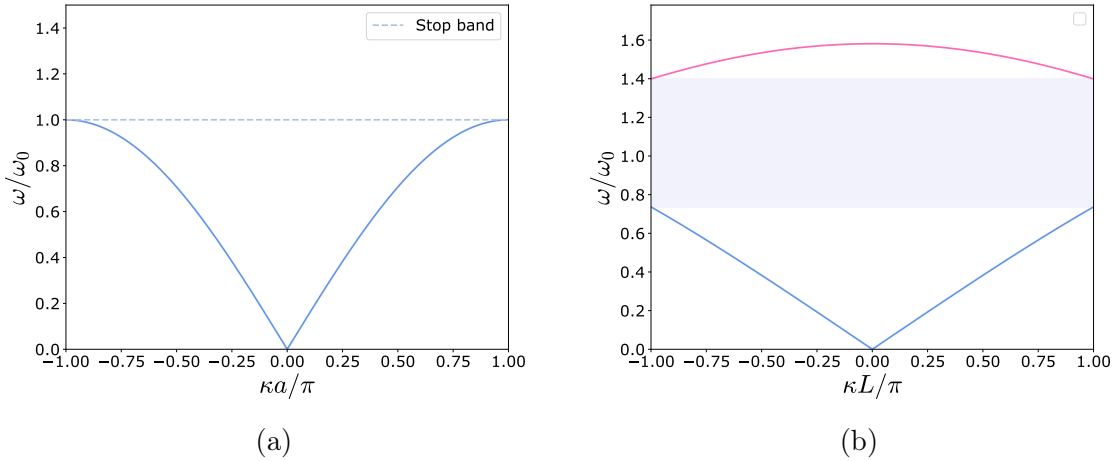


Figure 1.3: Dispersion relations for (a) a monoatomic lattice with lattice constant a , (b) a diatomic lattice with lattice constant $L = 2a$. Due to the difference in mass between the atoms, in (b) a bandgap is generated.

Dispersion curves provide information on the relation between frequencies and wavenumber, that is, between the temporal and spatial periodicity of a travelling wave. They can be employed to characterise the dynamical behaviour of a system a priori, to gain information of its responses. For two dimensional lattices, the equation of motion of a local, single mass unit cell can be written considering the connections to the neighbours given in the chosen Bravais lattice.

$$m\ddot{x}_{(0,0)} = k \sum_{i,j=1}^N (x_{(i,j)} - x_{(0,0)}) \quad (1.25)$$

with N number of connected elements and $i, j \in \mathbb{N}$ their indexes.

Considering an out of plane motion and plugging in the plane wave solution as in equation 1.19, the dispersion surface can be retrieved by solving for $\omega(\kappa_x, \kappa_y)$.

As it can be more complex to read the wave propagation information on a surface instead of a curve, it is usual to plot the dispersion relation along the contour of the so-called Irreducible Brillouin Zone (IBZ), as will be shown in next subsection.

The number of degrees of freedom inside an elementary cell equals the number of branches in the dispersion curve and the number of passing bands of the structure, for lattices in any dimension.

In continuous systems, equation 1.13 does not apply, thus the solution for each point x reads

$$x_n(x_1, t) = e^{i(\omega t - \kappa x_{n,eq})} \quad (1.26)$$

thus, from 1.22

$$c^2 \kappa^2 e^{i(\omega t - \kappa x_{n,eq})} = \omega^2 e^{i(\omega t - \kappa x_{n,eq})} \quad (1.27)$$

leading to

$$\omega = c|\kappa| \quad (1.28)$$

which is a linear relation, and thus refers to *non-dispersive* media.

1.1.5.1 Irreducible Brillouin Zones (IBZ)

The dispersion relation for a two-dimensional lattice can be plotted on a curve by considering the reduced wavenumber κ_r along the irreducible Brillouin zone (IBZ). The IBZ is the area enclosed by the high symmetry points, which can be determined by analysing the symmetries of the unit cell of the periodic structure. The high-symmetry points, namely Γ, X, M in the example cases, are displayed in table 5.1 for the different crystallographic groups, i.e. for the five types of Bravais lattices in two-dimensions, where the square and the rectangular lattices have a four-side polygon as first Brillouin zone, respectively with $b_1 = b_2, b_1 \neq b_2$, while the hexagonal, rhombic and oblique lattices have a six-sided one.

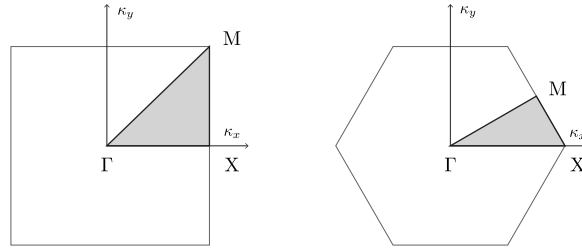


Figure 1.4: Irreducible Brillouin Zones (IBZ) illustrated for the square and rhombic lattices.

The reduced wavenumber κ_r path along the IBZ contour is obtained by connecting the high-symmetry points, and the dispersion relation becomes a curve with expression $\omega = \omega(\kappa_r)$.

1.1.6 Evanescent waves

Evanescent waves are solutions of wave equations in which the amplitude decreases exponentially with distance, without carrying energy. Unlike propagating waves, where energy is transferred through space, evanescent waves remain localized. In fact, these waves emerge in regions of the dispersion relation where $\omega > \omega_{cut-off}$, where the energy stops propagating but the lattice is not completely inert. The amplitude of an evanescent wave decreases exponentially as a function of the distance from the source, as the exponential function has a real, negative exponent.

An evanescent wave can be thus described through a complex wave number $\kappa = Re\{\kappa\} + iIm\{\kappa\}$, where the imaginary part determines the decay rate. Therefore the wave solution becomes:

$$x(x_1, t) = \Omega e^{i(\omega t Re\{\kappa\} x_{n,eq})} e^{Im\{\kappa\} x_{n,eq}} \quad (1.29)$$

where Ω is the amplitude and $e^{Im\{\kappa\} x_{n,eq}}$ describes spatial attenuation.

In phononic crystals and metamaterials, evanescent waves manifest within band gaps, where propagating waves are prohibited. Moreover, they often occur at discontinuities or interfaces, such as mirrors or waveguides.

1.1.7 Two to one atom unit cell

As in the mathematical treatment by Brillouin [8], a diatomic lattice with an unit cell with masses m_1, m_2 can be reduced to a monoatomic lattice in three ways:

$$\begin{aligned} m_2 &\rightarrow 0 \\ m_1 &\rightarrow \infty \\ m_1 &\rightarrow m_2 \end{aligned} \quad (1.30)$$

The first and the second case do not involve a change in the unit cell length and periodicity, and leads in the first case to the upper branch becoming higher and narrower until its disappearance, and in the second case to a single frequency $\omega = \omega_2$ being present, involving the motion of the sole lighter masses, with the heavier ones acting as restoring force. The third case will be discussed later in part two, and involves a change in the lattice periodicity from d to $d_1 = d/2$. The dispersion relation is a periodic curve, where the fundamental interval is contained in the interval $\kappa \in [-\pi/a, \pi/a]$, with a being the lattice unit distance. When the switch from a diatomic to a monoatomic lattice takes place due to the quality of the masses values $m_1 = m_2$, then the fundamental interval doubles in size. Furthermore, the dispersion relation features two curves in the diatomic case, with the band gap between them when the masses are equal. Therefore, a unitary curve must be restored when passing from a diatomic to a monoatomic configuration, since

$$m_1, m_2 = m = 2\sqrt{\frac{m_1 m_2}{m_1 + m_2}} \quad (1.31)$$

then

$$\omega^2 = \frac{k}{m} \left[1 \pm \sqrt{1 - \sin^2 \kappa_1} \right] = \frac{k}{m} (1 \pm \cos \kappa_1) \quad (1.32)$$

and from trigonometric bisection formulas

$$1 \pm \cos \kappa_1 = \begin{cases} 2\sin^2 \kappa_1/2 \\ 2\cos^2 \kappa_1/2 \end{cases} \quad (1.33)$$

The sine functions corresponds to the monoatomic dispersion relation in equation 1.24

$$\omega = 2\sqrt{\frac{k}{m} \sin^2 \kappa_1/2} \quad (1.34)$$

while the cosine function overlaps the curve, and its upper part replicates the upper curve of the diatomic case. Their intersection represents the limit of $\omega_1 = \omega_2$, and naturally no band gap is present.

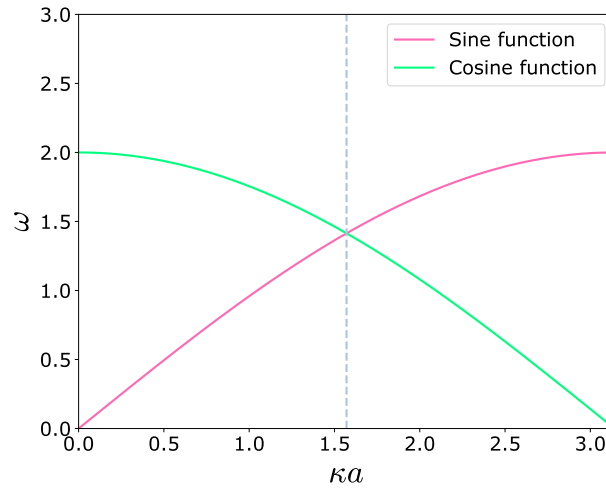


Figure 1.5: The plot shows the curve retrieved when the masses m_1, m_2 are equal. The sine curve, in pink, reaches the end of the newly found first Brillouin zone length, that goes from $\pi/2a$ to π/a when the unit cell halves in size, i.e. when it contains only one mass instead of two as in the diatomic chain. The cosine curve, in green, is the reflected representation of the dispersion curve in a smaller Brillouin zone.

1.1.8 Analytical and numerical methods

When the study of wave propagation concerns more complex geometries, or the system is finite, i.e. the periodic boundary conditions cannot be applied to reduce the analysis to the unit cell, band diagrams are obtained through several methods (analytical and numerical) that provide accurate approximations of the wave behaviour. First, a commonly employed analytical method is the plane wave expansion (PWE) [9]. This method yields the displacement field for periodic systems through Fourier analysis, by superimposing harmonics. In a similar fashion, the harmonic balance method (HBM) can be employed to retrieve the dynamical response of both periodic infinite and finite systems through Fourier analysis. The application to nonlinear differential equations with a wave form solution is discussed by Krack [10]. Another method that can be employed in the analysis of periodic systems is the transfer matrix method (TMM), based on the continuity at interfaces. Other common approaches to studying complex dynamical problems involve direct numerical simulations through the finite element method (FEM) ([11], [12]), or the spectral element method (SEM) [13]. Explicit numerical simulations of simple configurations with finite domains can be carried out through Newmark [14] and Runge Kutta 4 methods, respectively for the linear and nonlinear case, and numerical dispersion diagrams can be attained through two-dimensional fast Fourier transforms (2DFFT), which shift the results from time to frequency domain. Complex geometries and coupling with regular materials [15] can be computationally challenging to analyse, therefore homogenization techniques often come into play [16]. These methods are based on the concept that an infinitely large periodic metamaterial can be substituted with a homogenized continuum, replicating its behavior without considering all the intricate details of its microstructures.

1.1.9 Infinite to finite lattices

The theoretical presentation above refers to infinite systems, however in physical devices and samples the number of unit cells generating the lattice is limited. Unbounded domains are studied with Bloch-Floquet analysis, however it is possible to retrieve the dynamical response for finite systems in the

frequency domain through numerical techniques. In fact, the natural frequencies and mode shapes of the truncated system are anyhow to be found on the dispersion curves or surfaces. Vibration modes can be identified in correspondence with travelling waves on the graph, albeit not continuously for every wavenumber. The number of natural frequencies, in fact, corresponds to the number of degrees of freedom in the considered lattice, and their positioning on the dispersion curve depends on the boundary conditions of the system. For a ring topology the periodic Bloch-Floquet solution is deemed valid, while for free-free or fixed-fixed configuration the unit cells at the boundaries of the lattice do not obey the periodicity condition. However, the bulk of the system does and this ensures the possibility of a translation from an infinite periodic to a finite configuration. As discussed later in Chapter 1 and in Chapter 2, nonlocal configurations impact the size of the area to be considered boundaries in order to retrieve the analytically predicted behaviour.

1.2 State of the art: dynamics of nonlocal lattices

The mathematical formulation of long-range interactions in continua, both in statics and dynamics, can be expressed through both spatial differentiation and integration.

One of the fundamental contribution to nonlocal mechanics comes from Eringen ([17], [18]). The author's approach to non-local interactions involves several axioms which refer to the concept of *neighbourhood*. The neighbourhood dictates how the influence of distant material points affects a specific location. This can be mathematically expressed either through a *smooth* neighbourhood, where Taylor expansions of motion and temperature are assumed, leading to gradient-type materials. Another option is the *attenuating* neighbourhood, which introduces an influence function that diminishes the impact of distant points.

The group of Di Paola et al. ([19], [20]) utilises a mechanically based approach to non-local elasticity, modelling non-local effects through long-range interactions between material points. The interactions are considered as additional forces that are proportional to the interacting volumes and the relative displacements between them. A distance-decaying function to determine how these interactions diminish with distance is incorporated, typically a power-law, while the increasing of stiffness with distance is not taken into account. Mathematically, the approach uses integro-differential equations to describe elastic equilibrium, with kinematic restrictions accounting for relative displacements and constitutive equations relating stress and strain to long-range interactions. A variational formulation results in a potential energy functional, and when power-law decaying interactions are present, fractional calculus is employed, leading to equations with fractional derivatives.

Other authors investigate nonlocal elasticity through nonlocal integral constitutive laws. Among them, Romano et al. [21] focus the relation between stress and strain in materials at the nanoscale, especially in nano-beams, using nonlocal integral constitutive laws. These laws account for the dependence of the stress in a certain point depends not only on the strain in that point, but also on strains in other points in the material. Mathematically, this requires the usage of functional analysis through integral convolutions, where an averaging kernel weights the contribution of strain at different locations to determine the stress in a specific point. The boundary effects are one of the key issues discussed in their work. Averaging kernels used in the integral convolutions are designed for infinite domains, which do not accurately represent the long-range interactions of finite objects. To address this, the authors investigate compensation procedures that modify the kernels to account for the boundary effects, such as writing kernels as probability densities.

Another possible mathematical treatment of nonlocal interactions in dynamical models was proposed by Silling [22], through his theory of peridynamics. The peridynamic model allows particles separated by a finite distance to interact, in contrast with classical continuum mechanics, which primarily considers interactions between immediately adjacent particles. The distance at which the particles can interact is defined peridynamic *horizon*, i.e. the maximum distance at which two ele-

ments can directly influence each other. The peridynamic formulation uses integration to compute the forces acting on a material particle, rather than spatial differentiation. In fact, by avoiding spatial derivatives, the peridynamic equations remain valid even at points or surfaces of discontinuity, such as cracks, which is a key advantage to this modelling approach.. In fact, long-range forces are particularly important in applications like thin film mechanics, where fractures can easily arise.

Nonlocal interactions in discrete, periodic systems have instead garnered the interest of the scientific community only very recently, and have applications which significantly differ to those of the above-mentioned models.

1.2.1 Roton-like metamaterials

Roton-like metamaterials represent an advanced frontier in wave manipulation research, because they allow for backwards propagating waves and zero group velocity (ZGV) modes to emerge. They are inspired by quantum phenomena observed in superfluids at low temperatures, such as He^4 . In fact, the dispersion relations of these superfluids exhibit a non-monotonic curve, with energy decreasing with the increase in momentum. This is due to a relative rotation between the particles in specific regions, which reduces their momentum ([23], [24]).

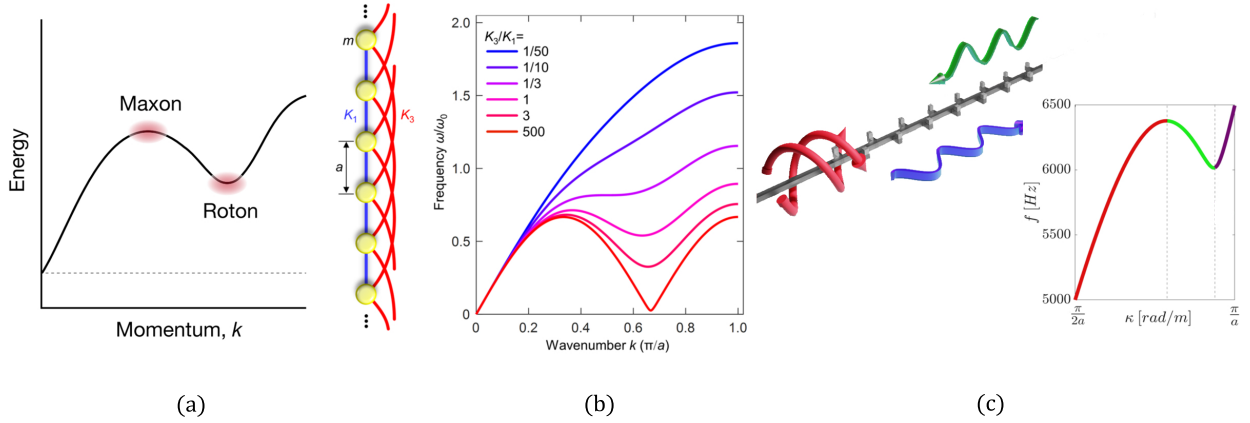


Figure 1.6: Adapted from the works of Park et al. [25], Chen et al. [26] and Iorio et al. [27]. Figure 1.6 (a) shows Landau's energy-momentum dispersion curve for the excitation spectrum of liquid helium 4, Figure 1.6 (b) shows the dispersion curves of a nonlocally connected monoatomic chains, varying with the ratio between the stiffness on the nonlocal and the local links, Figure 1.6 (c) shows the prototype of a metamaterial supporting three wave modes which yield a non-monotonic dispersion curve.

The history of rotons begins with Lev Landau, a Soviet physicist who proposed his theory of the superfluidity of helium-II [28] in 1941. Landau hypothesized the existence of two types of elementary excitations in this superfluid: phonons, with a monotonic dispersion relation, and rotons, characterized by a minimum of energy corresponding to a certain value in momentum. This is illustrated in Figure 1.6 (a), which shows the relation between energy and momentum.

Later, Richard Feynman provided a microscopic interpretation of Landau's theory, suggesting that rotons were associated with "return flow vortices" in the superfluid. Feynman and Cohen in 1956 published a fundamental study [29] on the energy spectrum of excitations in liquid helium.

Landau and Feynman's theoretical predictions were later experimentally verified through neutron scattering experiments. These experiments demonstrated the validity of the roton-like dispersion relationship, confirming the existence of rotons as fundamental excitations in superfluid helium.

Roton dispersion relations were previously confined to correlated quantum systems at low temperatures. However, recent studies reveal that this unique dispersion can also be achieved in acoustic and

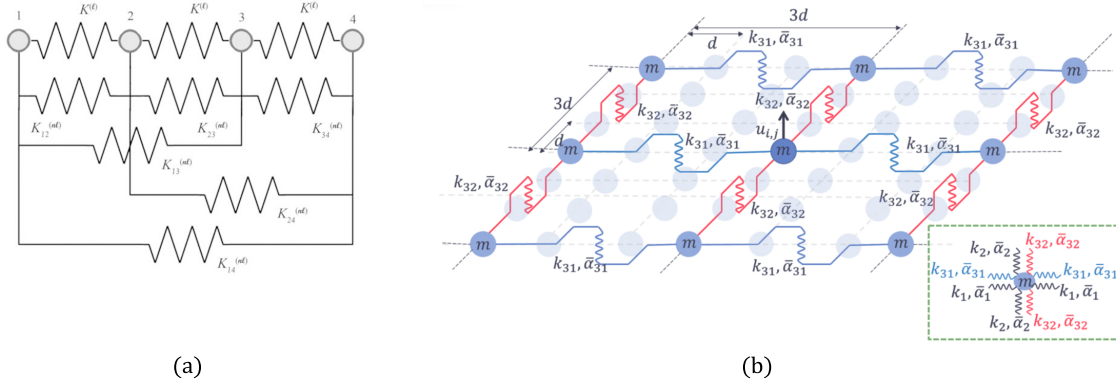


Figure 1.7: Figure adapted from the works of Cottone et al. [20] and Sepehri et al. [30]. Figure 1.7 (a) shows a discretised equivalent model used to study nonlocal interactions in continua, whereas Figure 1.7 (b) displays a simplified two-dimensional mass-spring model for slab nonlocal metamaterial design.

elastic metamaterials. This phenomenon has been observed in periodic structures through the implementation of interactions beyond nearest neighbors, based on the formulation originally developed by Brillouin in the 1950s.

Throughout the past three decades, a broad scientific community has invested time in developing artificial periodic lattices, i.e. metamaterials, with the scope of manipulating electromagnetic, elastic and acoustic waves. In this context, the idea of creating metamaterials with roton-like dispersion curves lends itself to manipulating waves in unconventional ways, which opens up novel possibilities for technological applications. The interest lies in obtaining anti-parallel phase and group velocities, with energy flowing opposite to the wavefront. The gap between obtaining non-monotonic dispersion curves in correlated quantum systems at low temperatures and macroscale systems has however been filled in the last century, as this phenomenon has been observed in periodic structures through the implementation of beyond nearest neighbour (BNN) interactions, firstly proposed by Brillouin in the '50s [8]. Furthermore, for interactions involving the N^{th} , $N - 1$ extrema will be generated in the first Brillouin zone. The nonlocal, long-range interactions are not tied to a specific type of links, as they can be implemented by means of elastic connections ([26],[31],[32]), electrostatic or magnetic forces. As a matter of fact, this was known since the 1960s in the electric engineering field [33].

Therefore, in order to achieve a roton-like dispersion in an elastic metamaterial, it is common practice to introduce various degrees of BNN interactions. The strength of the long-range interactions rules over the shape of the dispersion curve, as displayed in Figure 1.6 (b), where a mass spring chain supporting longitudinal vibration modes has monotonic or non-monotonic curve depending on the value of the 3^{rd} BNN connection, and when the local interaction becomes negligible shows the halving of the first Brillouin zone [26]. However, a roton-like dispersion can be achieved by coupling counterpropagating modes, without the need for interactions BNN neighbours, as illustrated in [27]. The proposed method employs coupling of different wave modes supported by elastic media, which can differ in wavelength, polarisation and velocity [4]. The prototype envisaged by the authors is shown in Figure 1.6 (c), where torsional (red), flexural in-plane (green) and flexural out-of-plane (blue) are coupled.

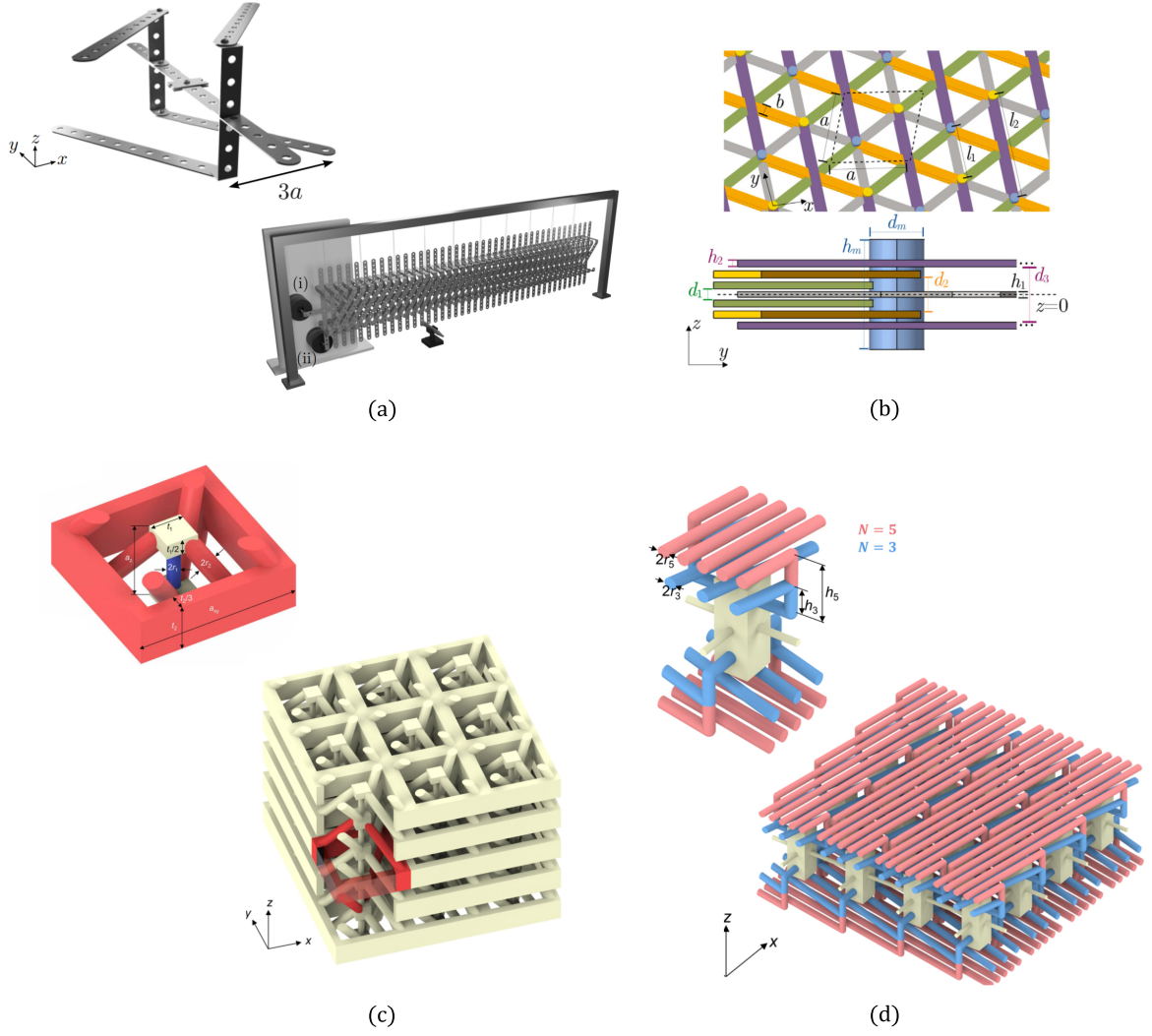


Figure 1.8: Figure adapted from the works of Chaplain et al. [31], Dal Poggetto et al. [34], Iglesias Martinez et al. [35] and Wang et al. [36]. Figure 1.8 (a) displays the nonlocal metamaterial sample built out of Meccano elements ideated by the authors. Figure 1.8 (b) shows a prospective experimental model for a two-dimensional lattice with out-of-plane displacements. Figure 1.8 (c) shows the experimental sample design of the authors, then translated both to the macro- and microscale. Finally, Figure 1.8 (d) shows a possible two-dimensional metamaterial slab design with nonlocal interactions and channels for pressure wave support.

Typically, metamaterial design is first conceived in a simplified analytical fashion, which allows for grasping the main working principle of the envisaged device. For elastic and acoustic waves, mass-spring models with long-range interactions are employed ([26],[31],[35],[37], [34], [32],[30],[38]). This is not new to metamaterial design, nor to nonlocal continuum systems. For instance, mass-spring models were employed by Cottone et al. [20] to study an integro-differential problem through a representation with an equivalent mechanical model. The fractional differential equation can be, in fact, converted into a discrete version using a difference operator, resulting in a system of ordinary differential equations, which corresponds to the equilibrium equations of a mass-spring model, where the local and non-local stiffnesses are determined by the parameters of the fractional differential equation. The simplified model is illustrated in Figure 1.7 (a), while in Figure 1.7 (b) the two-

dimensional simplified lattice model used to study nonlocal connections by Sepehri et al. is illustrated [30].

The translation from the simplified models to three-dimensional, tangible prototypes is often not trivial. In fact, attention should be paid to intersections between the links, material choice and testing environment conditions. Most importantly, the theoretical predictions and numerical simulations often involve infinite periodic structures with Bloch-Floquet boundary conditions, while in experimental setups finite lattices and boundary effects, especially important in nonlocal lattices, must be taken into account. Some theoretical and experimental examples from literature are gathered in Figure 1.8. The designs support several wave types, obtaining roton-like dispersion relations on at least the acoustical branch of the curve, i.e. the lowest, and at least on a path connecting two points on the IBZ path. Figure 1.8 (a) depicts the reconfigurable model by Chaplain et al. [31], who employ Meccano - a popular British toy- elements to build long-range interconnected elements. The structure uses a central strip for nearest-neighbor coupling and connecting strips for BNN coupling, and repositioning of such links allows for swapping the nonlocal connections. The incorporation of BNN coupling leads to multiple extrema within the first Brillouin zone. The sample is excited using a mechanical shaker, driven by a variable-frequency signal generator. The experimental measurements are retrieved by a microphone recording acoustic pressure fluctuations instead of direct measurements of the elastic fields. The work shows that numerical and experimental data are in good accordance with the analytical predictions, even though a finite model is tested. Another experimental work was carried out by Iglesias Martinez et al. [35], on the basis of a previous study of their research group [26]. Direct observation of roton-like dispersion relations is made on two three-dimensional metamaterials design, respectively at the micro- and macroscale. The metamaterials are based on an achiral tetragonal-symmetric structure. The designs involve small cubic volumes acting as atoms, with short cylindrical rods and channels mediating nearest-neighbour interactions and other beams/channels mediating third-nearest-neighbour interactions, as illustrated in Figure 1.8 (c). The strength of the interactions is determined by the length and cross-section of the cylindrical elements. Microscale samples were excited using a piezoelectric actuator, and nanometric displacement vectors were obtained through optical image digital cross-correlation analysis, whereas macroscale samples were excited using a loudspeaker, and local air-pressure modulation was recorded by a microphone in each unit cell. In both cases, the experimental data for both metamaterial designs agree with the numerical calculations performed, and roton-like curves are to be found in the lowest (acoustical branch) of the dispersion relations. Prospective experimental models for two-dimensional metamaterial wave filters are instead shown in Figures 1.8 (b) and (c). The model by Dal Poggetto et al. [34] in Figures 1.8 (c) is a potential experimental realisation of a hexagonal unit cell with third nearest neighbour connections and out-of-plane displacements. It is composed by cylinders (masses in the unit cell of the discretised model), which allow for multiple nonlocal links through flat elements insisting on their lateral surface. Finally, Figure 1.8 (c) displays the imagined metamaterial sample in the work of Wang et al. [36], in which the authors envisage a flexible two-dimensional metamaterial slab to tailor the lowest acoustical phonon dispersion relation for airborne sound, by using BNN interactions along two orthogonal directions. The long-range interactions are designed using a network of cylindrical tubes connecting cuboid compartments in a two-dimensional square array.

1.2.2 Aims of the study

This thesis focuses on establishing a design framework for nonlocal dynamical systems, based on their simplest paradigm, i.e. mass-spring models, in the form of periodic monoatomic and diatomic one-dimensional chains and two-dimensional monoatomic lattices.

The foundation of the proposed design framework lies in the realization that nonlocal discrete models present an inaccuracy in the dynamical formulation. In fact, when considering a mass-spring model, the mass of the links is neglected from the inertial contribution. However, when the number

of these connections increases, their mass becomes comparable to that of the atoms, therefore making the hypothesis of neglectable springs' mass in the dynamics no longer valid. A *mechanical consistency* condition is thus here enforced, in order to ensure a coherent dynamical response of the imagined nonlocal model. This concept is applied through a general rule, ensuring that the ratio between the masses of the springs and the point-wise masses is small, i.e. there is at least one order of magnitude separating their values. This translates to an a priori definition of the material masses at play, which comply with this condition, and that are only later subdivided into the envisioned linking conditions. This allows for different dynamical systems to be attained from the very same amount of mass to be distributed, always following the established principle. Moreover, this allows for an effortless comparison of local and nonlocal models, as their behaviour will be linked to the mass allocation among the local and nonlocal links. In Chapter 2, the above-mentioned *mechanical consistency* condition is formulated. A simple monoatomic one-dimensional spring model is considered to establish the general principles, without loss of generality. Two parameters ruling over the transition from local to nonlocal models are introduced, and the governing equations of the problems are subsequently reformulated on the basis of said parameters. In Chapter 3, the mass-conserving model is extended to a diatomic configuration, through an odd distribution of mass between two subsequent unit cells. The disparity of distribution could involve the masses of the atoms or those of the links, and in both cases a diatomic unit-cell emerges. The goal of this work is to observe how a *defected* configuration with a dishomogeneous mass distribution influences band-gap formation and width. In Chapter 4, a reasoning on an extension of the *mechanical consistency* condition is applied to weakly nonlocal chains, with the effort of expanding the formulation through suitable hypotheses. In Chapter 5, the goal is to study the influence of bidimensional connections and lattice geometries on wave propagation in nonlocal systems. Finally, some overall results and perspectives are discussed.

Chapter 2

Local-to-non-local transition laws for stiffness-tuneable monoatomic chains preserving springs mass

Abstract

Recently, nonlocal configurations have been proposed by adding beyond nearest neighbour couplings among elements in lattices to obtain roton-like dispersion relations and phase and group velocities with opposite signs. Even though the introduction of nonlocal elastic links in metamaterials has unlocked unprecedented possibilities, literature models and prototypes seem neither to provide criteria to compare local and nonlocal lattices nor to discuss any related rules governing the transition between the two configurations. A physically reasonable principle that monoatomic one-dimensional chains must obey to pass from single- to multi connected systems is here proposed through a mass conservation law for elastic springs thereby introducing a suitable real dimensionless parameter α to tune stiffness distribution. Therefore, the dispersion relations as a function of α and of the *degree of nonlocality* P are derived analytically, demonstrating that the proposed principle can be rather interpreted as a general mechanical consistency condition to preserve proper dynamics, involving the spring to bead mass ratio. Finally, after discussing qualitative results and deriving some useful inequalities, numerical simulations and 2D FFTs are performed for some paradigmatic examples to highlight key dynamics features exhibited by chains with finite length as the parameters α and P vary.

2.1 Introduction

Beyond nearest-neighbor (BNN) interactions are relevant in many fields of physics. In condensed matter physics, next-nearest-neighbor interactions have significant influence on the material properties as it is the case, for instance, of graphene, a two-dimensional material made up of carbon atoms arranged in a hexagonal lattice, which leads to nonlocal electronic hoppings [39]. The influence of long range couplings on the dispersion characteristics and dynamical response of 2D and 3D lattices is considerable, as the strength of interaction forces impacts wave and energy propagation ([40], [41], [42]).

In electromagnetism the concept has paved the way to potential waveguiding applications, especially in optics, that is in the visible range of electromagnetic wave frequencies ([43], [44], [45], [46]). Dynamical processes in classical mechanics can be influenced by BNN interactions as well. Their counterparts in statics have been extensively studied in the past, and both continuous ([18], [47]) and discrete [48] models have been analysed since the first contributions. Nonlocal elastic models in continua discussed in classical literature works, as in the works by Eringen et al. ([49], [17],[18]), present

the challenge of adapting the constitutive stress-strain relationship of nonlocal classes of materials, so that their constitutive response be attenuated with distance between two arbitrarily distant points. For this purpose, the authors introduced an influence function with an exponential law to ensure the decay of the elastic moduli along with the distance between the given points.

More recently, alternative nonlocal models have been proposed for elastic and fracturing nonlocal metamaterials. Peridynamic models are among these, as the bond-bond ones proposed by Silling [22], where a power law is employed with the aim of decreasing the links' stiffness when farther from the so-called peridynamic horizon.

A few real materials are known to exhibit a nonlocal microstructure. A 2D existing man-made material with evidence of nonlocal organization is constituted by some types of recycled or cold-pressed sheets of paper, in which connections and entanglements of intricate network of linear elastic filaments can be recognized at microscopic level and influence their fracture mechanisms.

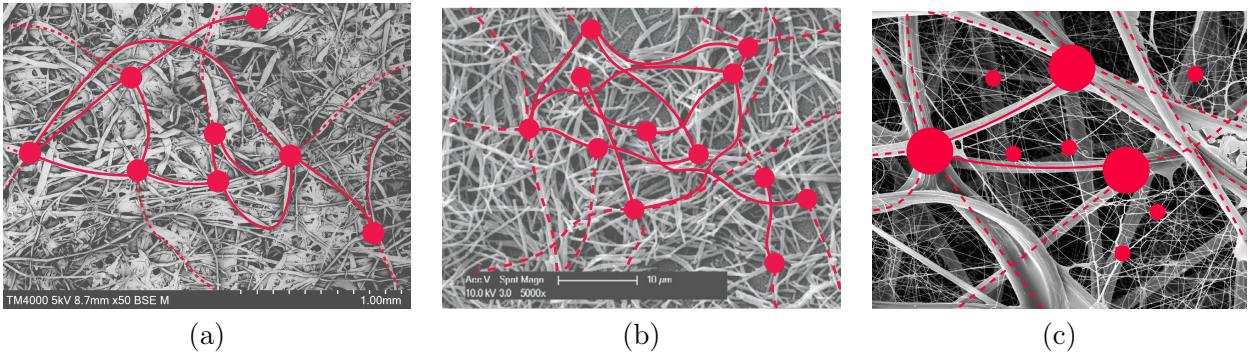


Figure 2.1: In the Figure above three materials exhibiting a nonlocal microstructure are shown through pictures taken by Scanning Electron Microscope (SEM), and adapted to highlight the nonlocal links. In (a) a scan of rice-paper is shown in a capture performed at the lab LIMiTS of the University of Naples Federico II with SEM Hitachi series TM4000 plus. The paper is composed by cold-pressed sheets with several nonlocal links. In (b) a SEM scan from Kim et al. [50] is adapted, where polydiethylfluorene nanorods are interlaced and nonlocally paired. Finally, in (c) a SEM image of spider silk from <https://www.sciencephoto.com/media/373522/view/spider-s-web-sem> is overlapped by a scheme that highlights the multiple, hierarchical nonlocal connections.

Nonlocal pairings can furthermore be observed in nanorods of different elements [50], in spider silk and in polymer entanglements. Due to their nonlocality, these materials have encouraged the development of several nonlocal models in statics and dynamics, both in the continuum and discrete domain through different approaches, from constitutive boundary conditions to peridynamics, to fractional models. ([21], [51], [52],[20]). From Figure 2.1 the nonlocal sub-structure of some of the materials cited above can be observed through Scanning Electron Microscope images, on which a possible simplified scheme of the pairings has been illustrated.

In the latest years the topic has gained attention of the researchers due to its potential breeding with metamaterial design and thus its role in wave propagation, localization or energy harvesting. In fact, tunability and shifts in the frequency range are of utmost importance in metamaterial design, as they encompass a broad set of scales and applications. ([53], [54]). The seminal work by Brillouin [8] already takes into account nonlocal couplings in the theory of wave propagation in monoatomic lattices, and provides the dispersion relation for a set number of BNN couplings as early as in 1956. In the phononic crystals and metamaterials design field, the influence of BNN interactions can be of crucial importance in governing waves and thus energy propagation. As periodic structures they can be analysed through Bloch's theory, originally applied to crystalline structures [55], the overview of

their dynamical behavior can be read on a dispersion curve. Moreover, some studies were carried out to analyse the interaction forces in a nonlocal infinite periodic chain [38] and the response to the motion of one element [56]. The potential of nonlocally connected lattices in applications is tied to the resulting "roton-like" dispersion relation, which is peculiar because it has a curve presenting a local minimum, corresponding to an inversion of sign of the group velocity (velocity at which the wave packet and thus the energy moves, as opposed to phase velocity which corresponds to the velocity at which the wave front moves forward). This concept, which might seem fairly new in mechanics, has however a long history: in 1962 Landau was awarded the Nobel prize for identifying what he named "rotons" in the dispersion relations of superfluid 4He at low temperatures [28], that he predicted and Feynman observed in experiments on inelastic neutron scattering in 1961 [29]. The rotons are also observed in Bose-Einstein condensates, and they still represent an active research branch ([23], [57], [58]).

In recent years some studies ([59], [36]) have proven it possible to obtain the same kind of dispersion diagram experimentally in *ad hoc* designed phononic crystals and periodic metamaterials. In this case there is no contribution of quantum effects involved and no correlation to low temperatures, to great advantage of experimental stages. Possible applications can even mingle with other relevant topics in the metamaterials community, as topology and disordered lattices ([60], [61]), where they contribute to the appearance of localised modes. In mechanics, increasing the number of BNN interactions causes the local minima (corresponding to rotons) and maxima (corresponding to maxons) to increase accordingly ([62], [63]). Taking advantage of this feature to obtain specific dispersion curves, a very recent study by Kazemi et al. [63] produced a detailed method for tailoring specific dispersion relations through the usage of Fourier series coefficients as spring constants, proving how powerful a tool BNN interactions in metamaterials can be and to exploit some parameters to design curves fitting to certain goals of wave propagation and zero group velocity modes, going a step further by analysing their diffusion rate.

Interestingly, the roton-like behaviour in dispersion curves was proven not to be solely tied to BNN connections, but also to hybridization and/or polarization of modes in elastic, electromagnetic and acoustic waves ([64],[65],[66],[67],[68]).

Iglesias Martínez et al. [35] provided experimental proof of the roton-like dispersion relations in 3D metamaterials through BNN. Two different experiments were carried out, one with transverse elastic waves in microscale materials and ultrasound frequencies, the other with longitudinal air-pressure waves in macroscopic channel based materials at audible frequencies. They underlined how the real advantage of the BNN interactions are in tailoring the lower branch while the other metamaterial studies focused on tweaking higher branches. In [69] BNN is used to design a metamaterial with backwards propagating waves, i.e. with different signs in group and phase velocity. The numerical and experimental model is 3D, achieved through Meccano construction elements, which gives rise to a prototype with interchangeable pieces. In [30] Sepehri et al. examine the behaviour of the non-local phononic crystals when the nonlinearity comes into play. A monoatomic chain with 3rd BNN interactions is the reference model with roton-like dispersion relation and backwards wave propagation as a result. They introduce nonlinearity as a means of studying amplitude-dependent behaviour, which could enhance the tuneability abilities. A paper by Zhu et al. [70] focuses on multidirectional roton-like dispersion relations following the work from Chen et al. [59], by developing an experiment on roton-like dispersion relations in acoustical metamaterial at ambient temperature. In this manner backwards waves are obtained, in analogy to the return flow defined by Feynman [29].

A sound mechanical and physical foundation of the way in which the nonlocalities are devised is however generally missing in the majority of these models. In fact, a simple increase in couplings implies a variation in the overall stiffness and different scaling laws do not lead to a straightforward physical comparison between different models, being them local or nonlocal. Most importantly, a paradox could arise as most of the studies cited above perform their preliminary analyses on a mass-

spring model. In fact the main assumption in employing these simplified models is that the only masses who participate in the dynamics of the system are those of the atoms, while the springs' masses are considered negligible. However when the number of nonlocal pairings increases, the mass of the springs increases accordingly, and disregarding it in the dynamical analyses could lead to the model's inconsistency. An example of this contradictory case can be for instance imagined for a system as the one studied and actually manufactured as prototype by Park et al. ([71]). If one added up an arbitrary number of nonlocal springs to the flexural metamaterial model without preserving spring mass, the same springs' masses would rapidly become of the order of magnitude of the oscillating masses as the number of elastic connections increases: as a result, that raw material would be called into play participating to the dynamics, in clear contrast to the hypotheses that consider the springs' mass negligible.

The present study explores the various implications of enforcing additional BNN couplings in a scenario where the amount of material is limited, and an order of magnitude ratio is enforced between the springs' and the atoms masses. Thus, a novel mass conservation law is proposed, in which a stiffness distribution parameter α rules the nonlocality of choice of the system and the dispersion characteristics. In this manner a rational comparison can be made between local and nonlocal models, on the basis of a different distribution and arrangement of the same amount of material, which is a common occurrence in designing any structural component and may be thus reasonably applied to metamaterials.

With the aim of gaining some insights into how nonlocal elasticity might contribute to suggest new optimization strategies for designing 1D structures and possibly three-dimensional lattices and metamaterials, the work makes reference to the simplest paradigm of a mono-atomic chain made of masses equally distanced between each other and mutually connected by linearly elastic springs. Dispersion relations for such 1D systems are then obtained and the dynamic response of selected case studies is analysed by forcing the mass (or equivalently the volume) of the elastic links branching off from each single mass to be constant.

This paper is structured as follows: in Section 1 a basic overview of the physical principles and mathematical methods behind the analysis of a nonlocal one-dimensional monoatomic chain is provided; in Section 2 the proposed mass-conservation constraints are introduced and a numerical simulation of the behaviour of the model in a finite chain scenario is presented, thereafter the consequences of the introduced assumptions are investigated; in Section 3 the advantages and limitations of this approach are finally highlighted and discussed.

2.2 Modelling and analysis of nonlocal monoatomic chains

In this Section the proposed material constraint is presented, preceded by a swift summary of the mathematical tools employed in the study and their physical meaning. The implications of the adopted approach are then unfolded both through the theoretical framework cited above and explicit dynamics simulations.

2.2.1 Fundamentals on Bloch-Floquet monoatomic chains equipped with nonlocal springs

The classical 1D model of a monoatomic chain made up of an arbitrary number N of masses and $(N-1)$ springs is considered. The system is assumed periodic with Bloch-Floquet boundary conditions, with a unit cell repeating itself at the lattice length a .

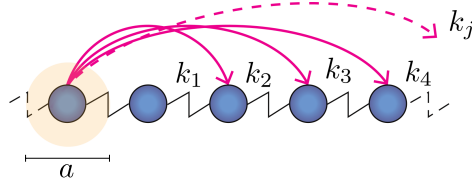


Figure 2.2: Scheme of the periodic nonlocal 1D mass spring chain. The highlighted area represents the unit cell, of length a , with its P number of connections with stiffness $k_1, k_2, \dots, k_j$ to the other unit cells at distance aj , which feature the same connections to the neighbours.

To characterize such dynamic system, the energy–momentum dispersion relation –written in terms of frequency against wavenumber– has to be first derived. Exactly as in the standard case of local chains, by writing the equilibrium through Newton’s 2nd law for the generic n^{th} mass and neglecting viscous contributions, one writes

$$F_n = m\ddot{x}_n = \sum_{j=1}^P k_j(x_{n-j} - 2x_n + x_{n+j}), \quad \forall n \in \{1, 2, \dots, N-1, N\} \subset \mathbb{N}, \quad P \in \mathbb{N} \quad (2.1)$$

where x_n is the actual position of the n^{th} mass and k_j is the stiffness of the spring connecting two masses distanced by $j-1$ elements (i.e. $j=1$ denotes local springs and $1 < j \leq P$ refers to nonlocal connections).

The solution to this equation is then obtained through Bloch-Floquet theory for periodic systems, which assumes a travelling wave solution with a phase factor as follows:

$$x_n = Ce^{i\omega t - i\kappa x_n^{\text{eq}}} = Ce^{i\omega t - i\kappa na} \quad (2.2)$$

$$x_{n-j} = Ce^{i\omega t - i\kappa x_{n-j}^{\text{eq}}} = Ce^{i\omega t - i\kappa(n-j)a} \quad (2.3)$$

$$x_{n+j} = Ce^{i\omega t - i\kappa x_{n+j}^{\text{eq}}} = Ce^{i\omega t - i\kappa(n+j)a} \quad (2.4)$$

where the apex eq refers to equilibrium position of the masses, C is an arbitrary constant representing the displacement amplitude, a is the unit cell length, κ is the wavenumber, the exponential form $e^{i\omega t - i\kappa x_n^{\text{eq}}}$ is the travelling wave and the periodicity indicates that the solution moving away from the unit cell varies by a factor $e^{i\kappa ja}$.

Inserting the solution into the equilibrium equation yields:

$$C \left[2 \sum_{j=1}^P (k_j - k_j \cos j\kappa a - m\omega^2) \right] = 0, \quad \forall C \in \mathbb{R} \quad (2.5)$$

so that, after some algebraic manipulations, the dispersion relation is given by

$$\omega = \omega(\kappa) = \sqrt{2m^{-1} \left(\sum_{j=1}^P k_j (1 - \cos(j\kappa a)) \right)} = \frac{2}{\sqrt{m}} \sqrt{\left(\sum_{j=1}^P k_j \sin^2(j\kappa \frac{a}{2}) \right)} \quad (2.6)$$

where the wavenumber κ is defined in the interval $[-\pi/a, \pi/a]$, corresponding to the length of the 1st Brillouin zone in the so-called reciprocal space or lattice, while it is worth to notice that the stiffnesses k_j are at this stage not yet explicitly given.

Key quantities like nonlocal monoatomic chain phase and group velocities can be also obtained. In fact, the dispersion relation provides information on the relationship between the angular frequency

of the waves ω and their wavenumber κ . In particular, the group velocity –the velocity at which the envelope of wave packets travels– is then defined as the derivative of the dispersion relation over κ , thus representing the slope of the above mentioned $\omega - \kappa$ graph and, in the present case, it takes the form:

$$v_{gr} = \frac{\partial \omega(\kappa)}{\partial \kappa} = \frac{a}{2\sqrt{m}} \frac{\sum_{j=1}^P j k_j \sin(j\kappa a)}{\sqrt{\sum_{j=1}^P k_j \sin(j\kappa \frac{a}{2})}} \quad (2.7)$$

As it is well-known, in such dynamical systems it is particularly important to compare the sign of the group velocity with that of the phase velocity v_{ph} , defined instead as the ratio of ω to κ , which in the case at hand takes the form:

$$v_{ph} = \frac{\omega(\kappa)}{\kappa} = \frac{2}{\kappa\sqrt{m}} \sqrt{\left(\sum_{j=1}^P k_j \sin^2(j\kappa \frac{a}{2})\right)} \quad (2.8)$$

which describes the rate of propagation of a component of the wave packet. When the ratio between the group and the phase velocity is negative, backwards-propagating waves take place, while instead when the group velocity is zero, zero group velocity modes appear and no energy is propagated through the lattice, both cases being fundamental for example for characterizing dynamics of metamaterials. It is worth noticing that, from the equations above, the study of the sign of the ratio of group and phase velocities can be helpfully reduced to analyse the following function sign

$$s \equiv \text{sgn}\left[\frac{v_{gr}}{v_{ph}}\right] \propto \sum_{j=1}^P j k_j \sin(j\kappa a) \quad (2.9)$$

limiting to consider its behavior in the symmetrical Brillouin hemi-region $\kappa \in [-\pi/a, \pi/a]$, once the explicit expression for stiffness k_j is provided.

2.2.2 The proposed *mechanical consistency condition* to govern local-to-nonlocal transition in BNN chains

The key idea of the present study is to set a framework to build BNN systems obeying the previous governing equations and characterized by various degrees of non-locality P , by prescribing necessary rules on the ratio between mass of material to be used respectively for the elastic springs and the atoms. This allows first of all to ensure mechanical consistency of the model when a large amount of nonlocal pairings are entailed and to compare and evaluate optimal configurations for different nonlocal chains, paving the way to establish design criteria and to envisage new paradigms for conceiving nonlocal metamaterials.

In order to do so, under the hypothesis of periodicity of the chain system, the proposed constraint keeps the total mass of the links converging in a given atom as constant, no matter how many BNN pairings are involved. In particular, the mass of each bead m is assumed constant, while the mass of the spring can be individually variable. In doing so, the inertia of the links, radiating out from that bead, must be regarded as negligible in order not to contribute to the dynamics of the chain. For this reason, a conservation law is here imposed to the total springs' mass m_s . Moreover, since density of the spring material ρ_s is considered constant, the proposed scaling can be consequently applied only to the total volume V_s of the elastic links afferent to the periodic unit cell, centered on the n^{th} atom. In addition, the length of every spring is considered as given by the distance between the two masses it connects, with a being the minimum length. Hence the proposed scaling law involves only the cross section of the links.

Assuming a certain value $V_s = V_{const}$ for the volume, and considering different levels of connection in the infinite chain, the volume balance of the unit cell of a chain with a P level of nonlocality reads

$$\sum_{j=1}^P A_j^{(P)} ja = V_{const} \quad (2.10)$$

where $A_j^{(P)}$ is the cross section of the j^{th} spring of a chain with a level of nonlocality P , so that whatever is the level of connection and, consequently, the number of link cross sections to be considered in the equation, the overall volume of the springs, i.e. the amount of mass, remains constant.

2.2.3 Hypothesis of power law for scaling elastic spring stiffness with distance

Once the conservation of mass for the elastic links is imposed, how springs stiffness scales with the inter-atomic distances remains unconstrained because the conservation equation, imposed in terms of constant volume V_{const} , involves P geometric quantities, the cross sectional areas $A_j^{(P)}$. To constrain these geometric parameters and to be able to solve the equation, a new equation is introduced. It assumes a sufficiently general power law for describing how stiffness needs to scale with distances, with a stiffness distribution parameter α spanning over both positive and negative values. The condition is

$$A_j^{(P)} = A_1^{(P)} j^{-\alpha}, \quad \alpha \in \mathbb{R} \quad (2.11)$$

where the exponential α is introduced as a *stiffness distribution* parameter imposed beforehand that will serve the purpose of increasing or decreasing the stiffness on a j^{th} nonlocal spring. This choice adds a second parameter to the model, so that setting both the level of nonlocality P and the stiffness distribution parameter α is required in order to control the model itself.

Substituting equation 2.11 in the volume conservation equation 2.10, for a generalised P^{th} next nearest interacting chain the cross-section of the local links is then defined through the α parameter as follows

$$A_1^{(P)} = \frac{V_{const}}{a \sum_{j=1}^P j^{1-\alpha}} \quad (2.12)$$

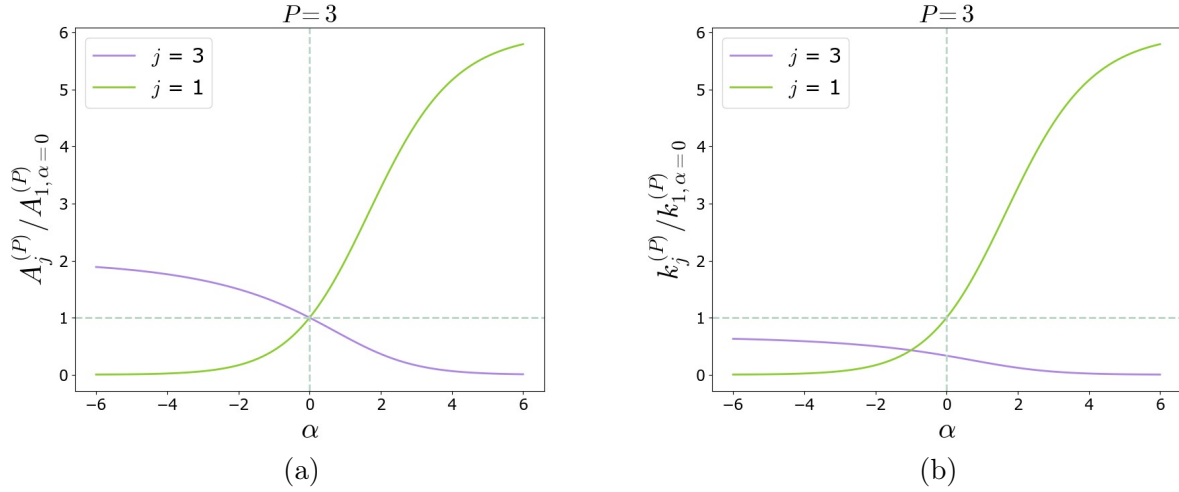


Figure 2.3: Considering a monoatomic chain with a level of nonlocality $P = 3$, the graphs shows how (a) $A_j^{(P)}$ and (b) $k_j^{(P)}$ vary for different α values in the most local and nonlocal springs. The values are normalised respectively over $A_1^{(P)}$ and $k_1^{(P)}$ calculated for $\alpha = 0$.

The stiffness of the springs is defined as

$$k_j^{(P)} = \frac{EA_j^{(P)}}{a_j} \quad (2.13)$$

where E is the Young modulus of the raw spring material, a_j is the length of the j^{th} link, which equals to ja , and $A_j^{(P)}$ is the corresponding cross section, in which the subscript indicates it connects the j^{th} next neighbour and the superscript denotes the maximum number of BNN connections in the designed chain.

In fact, for a mono-atomic (discrete) model of masses and springs with linear (local or nonlocal) and elastic interactions, every mass has one degree of freedom along the axis of the system and, therefore, the simplest way to connect elastically (nearest or beyond next nearest) masses is to assume linearly elastic prismatic bars with cross section area A and length L , from which the equivalent spring stiffness results as EA/L , where E is the Young modulus of the material.

$k_j^{(P)}$ can be defined as follows, from equations (4.18), (2.11) and (2.12):

$$k_j^{(P)} = \frac{A_j^{(P)} E}{a_j} = \frac{E}{a_j} \frac{A_1^{(P)}}{j^\alpha} = \frac{EV_{cost}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}}, \quad a_j = ja, \quad j \in \{1, \dots, P\} \quad (2.14)$$

In Equation (2.14) the stiffness distribution following the index of the BNN connected by the j^{th} spring and α is clear, as the sole non-constant value, once the values of E, V_{cost}, a, P and α for the chain are set, is $(j^{1+\alpha})$. Depending of the nonlocality level of the spring, its stiffness will depend on the α value selected. As $\alpha > 0$, the classical hyperbolic scaling law of stiffness with distance is recovered, while as $\alpha < 0$, unconventional albeit possible stiffness values that increase with inter-atomic distances are obtained.

Examples the ratio of $A_j^{(P)}/A_{1,\alpha=0}^{(P)}$ and $k_j^{(P)}/k_{1,\alpha=0}^{(P)}$ are presented in Figure (2.3). By varying the parameter α within the range of $\alpha \in [-6, 6]$, the effects on the cross section (Figure (2.3) (a)) and on the stiffness (2.3) (b)) of the P_{th} next-neighbour are observed. The green curves represent the area and the stiffness of the spring connecting the 3^{rd} BNN neighbour, and they have opposite concavities compared to the pink curves, which refer to the local connections. When the value of α increases, the

Chapter 2. Local-to-non-local transition laws for stiffness-tuneable monoatomic chains preserving springs mass

cross-section and the stiffness of the local links increase accordingly, while the nonlocal counterparts decrease. The opposite behaviour is observed when α assumes negative values.

2.2.4 Explicit dispersion relation, group and phase velocities

Once the mass conservation for springs is imposed and how elastic spring stiffness scales with distance is defined, some relevant quantities for describing the dynamics of nonlocal mono-atomic chains can be explicitly given.

In particular, from (4.3) the dispersion relation follows

$$\omega = 2\sqrt{\frac{EV_{const}}{ma^2}} \sqrt{\left(\sum_{j=1}^P j^{1-\alpha}\right)^{-1} \sum_{j=1}^P j^{-(1+\alpha)} \sin^2(j\kappa \frac{a}{2})} \quad (2.15)$$

Recalling the above mentioned discussion on the *mechanical consistency condition* and its relation with the admissibility of preserving arbitrary low spring to bead mass ratios, it is helpful to introduce this masses ratio explicitly as:

$$\mu = \frac{m_s}{m} = \frac{\rho_s V_s}{m} \equiv \frac{\rho_s V_{const}}{m} \ll 1 \quad (2.16)$$

which ensures that mono-atomic chain dynamics involves the oscillating atoms only, the inertial contribution of spring mass being negligible regardless of the number of elastic links and hence of the level of non-locality P . Recalling that elastic waves in the spring raw material travel at the speed v_s , it follows:

$$v_s = \sqrt{\frac{E}{m_s}} \implies V_{const} = \frac{\mu m v_s^2}{E} \quad (2.17)$$

from which the final dispersion relation can be effectively rewritten as

$$\omega = \frac{2\sqrt{\mu}}{\tau} \sqrt{\left(\sum_{j=1}^P j^{1-\alpha}\right)^{-1} \sum_{j=1}^P j^{-(1+\alpha)} \sin^2(j\kappa \frac{a}{2})}, \quad \tau = \frac{a}{v_s} > 0 \quad (2.18)$$

τ being a *characteristic time* of the system, representing the time spent by the elastic wave to travel inside the spring raw material to cover the minimum distance a between two near chain atoms. As the mass ratio μ , τ also plays a crucial role in describing the actual dynamics of such 1D systems, since it tells us about possible scattering or interference phenomena resulting from the competition between group and phase velocities and intrinsic (spring raw material) velocity v_s of elastic waves, running along the links of the chain nonlocal network.

This is why group and phase velocities are specialized to the case in which the stiffness coefficients k_j obey the conservation of mass (i.e. Equation (2.14)) and are respectively rewritten below as function of the parameters μ and τ as well

$$v_{gr} = \frac{\sqrt{\mu}}{2\tau} \frac{\sqrt{\left(\sum_{j=1}^P j^{1-\alpha}\right)^{-1} \sum_{j=1}^P \sin(j\kappa a) j^{-\alpha}}}{\sqrt{\sum_{j=1}^P j^{-(1+\alpha)} \sin^2(j\kappa \frac{a}{2})}} \quad (2.19)$$

and

$$v_{ph} = \frac{2\sqrt{\mu}}{\tau\kappa} \sqrt{\left(\sum_{j=1}^P j^{1-\alpha}\right)^{-1} \sum_{j=1}^P j^{-(1+\alpha)} \sin^2(j\kappa \frac{a}{2})} \quad (2.20)$$

Importantly, by means of some algebraic manipulations, it follows that the sign function can now be explicitly estimated as

$$s \equiv \text{sgn}\left[\frac{v_{gr}}{v_{ph}}\right] \propto \sum_{j=1}^P j^{-\alpha} \sin(j\beta\pi), \quad \kappa = \frac{\beta\pi}{a}, \quad \beta \in (0, 1) \quad (2.21)$$

where β was introduced to make reference to a dimensionless sign function to be studied in the symmetrical Brillouin zone of positive wavenumbers κ .

2.2.5 Some useful inequalities for nonlocal mono-atomic chains

The formulas obtained above allow to highlight some remarkable qualitative results.

One emerges from the analysis of the sign function (2.21), which plotted for $\beta \in [0, 1]$ and arbitrary integers P shows the important evidence that the group and phase velocities are always coherent, provided that α is greater than or equal to one, that is

$$\forall \alpha \geq 1, \quad s \equiv \text{sgn}\left[\frac{v_{gr}}{v_{ph}}\right] \geq 0, \quad \{\forall \beta \in [0, 1] \subset \mathbb{R}^+, \quad \forall P \in [1, +\infty[\subseteq \mathbb{N}\} \quad (2.22)$$

Within the framework of metamaterials to be designed for exhibiting opposite-in-sign group and phase velocities, this inequality gives a key information stating that, regardless the grade P of nonlocality, mono-atomic chains whose masses are connected with elastic springs that scale a in (2.14) can dynamically retrieve the roton-like behaviour if and only if the stiffness tuning parameter $\alpha < 1$.

Also, with in mind metamaterials exhibiting band gap, some universal as well as α -dependent upper bounds for frequencies ω can be found in the Brillouin zone from the obtained nonlocal dispersion relation.

A first general upper bound for ω can be derived taking advantage of the mathematical terms of the sums as follows:

$$\frac{\tau^2}{4\mu} \omega^2 = \frac{\sum_{j=1}^P j^{-(1+\alpha)} \sin^2(j\kappa \frac{a}{2})}{\sum_{j=1}^P j^{1-\alpha}} \leq \frac{\sum_{j=1}^P j^{-(1+\alpha)}}{\sum_{j=1}^P j^{1-\alpha}} \leq \frac{\sum_{j=1}^P j^{1-\alpha} j^{-2}}{\sum_{j=1}^P j^{1-\alpha}} \leq 1 \Rightarrow \omega \leq \frac{2\sqrt{\mu}}{\tau}, \quad \forall \alpha \in \mathbb{R} \quad (2.23)$$

from which no waves at frequencies over the obtained upper bound can travel in the mono-atomic chain, regardless the level P of nonlocality and independently from the way in which the stiffness of nonlocal springs is tuned with distance through the parameter α .

Another better upper bound for ω , finally given analytically as a function of α and P , can be found by exploiting the Cauchy-Schwarz inequality, but for $\alpha \geq 1$. In fact, being all coefficients in the sums non-negative terms, one first writes:

$$\frac{\tau^2}{4\mu} \omega^2 = \frac{\sum_{j=1}^P c_j(\alpha) j^{-2} s_j^2}{\sum_{j=1}^P c_j(\alpha)} \leq \frac{(\sum_{j=1}^P c_j(\alpha)^2 j^{-4})^{\frac{1}{2}} (\sum_{j=1}^P s_j^4)^{\frac{1}{2}}}{\sum_{j=1}^P c_j(\alpha)} \leq \frac{(\sum_{j=1}^P c_j(\alpha)^2)^{\frac{1}{2}} (\sum_{j=1}^P s_j^4)^{\frac{1}{2}}}{\sum_{j=1}^P c_j(\alpha)}, \quad \forall \alpha \in \mathbb{R} \quad (2.24)$$

where, for simplicity, we baptized c_j and $s_j(\alpha)$ as follows

$$c_j(\alpha) = j^{1-\alpha}, \quad s_j = \sin(j\kappa \frac{a}{2}) \quad (2.25)$$

By noticing that

$$\sum_{j=1}^P c_j(\alpha)^2 \geq 1 \Rightarrow \left(\sum_{j=1}^P c_j(\alpha)^2 \right)^{\frac{1}{2}} < \sum_{j=1}^P c_j(\alpha)^2, \quad \forall \alpha \in \mathbb{R} \quad (2.26)$$

it is possible to continue the chain of inequalities as follows

$$\frac{\tau^2}{4\mu} \omega^2 = \frac{\sum_{j=1}^P c_j(\alpha) j^{-2} s_j^2}{\sum_{j=1}^P c_j(\alpha)} \leq \frac{(\sum_{j=1}^P c_j(\alpha)^2)(\sum_{j=1}^P s_j^4)^{\frac{1}{2}}}{\sum_{j=1}^P c_j(\alpha)}, \quad \forall \alpha \in \mathbb{R} \quad (2.27)$$

Finally, if $\alpha \geq 1$, one has

$$\frac{\tau^2}{4\mu} \omega^2 = \frac{\sum_{j=1}^P c_j(\alpha) j^{-2} s_j^2}{\sum_{j=1}^P c_j(\alpha)} \leq \left(\sum_{j=1}^P s_j^4 \right)^{\frac{1}{2}} = \sum_{j=1}^P \sin^4 \left(j \kappa \frac{a}{2} \right), \quad \forall \alpha \geq 1 \quad (2.28)$$

from which, since the sum at the right hand has analytical expression, one has

$$\omega \leq \frac{\sqrt{\mu}}{2\tau} \sqrt{\frac{\sin(2a\kappa(2P+1))}{\sin 2a\kappa} - \frac{4\sin(a\kappa(2P+1))}{\sin a\kappa} + 6P+3}, \quad \forall \alpha \geq 1 \quad (2.29)$$

which provides a new upper bound for the frequencies related to nonlocal mono-atomic chains.

2.2.6 Effects of the stiffness tuning parameter α on the model

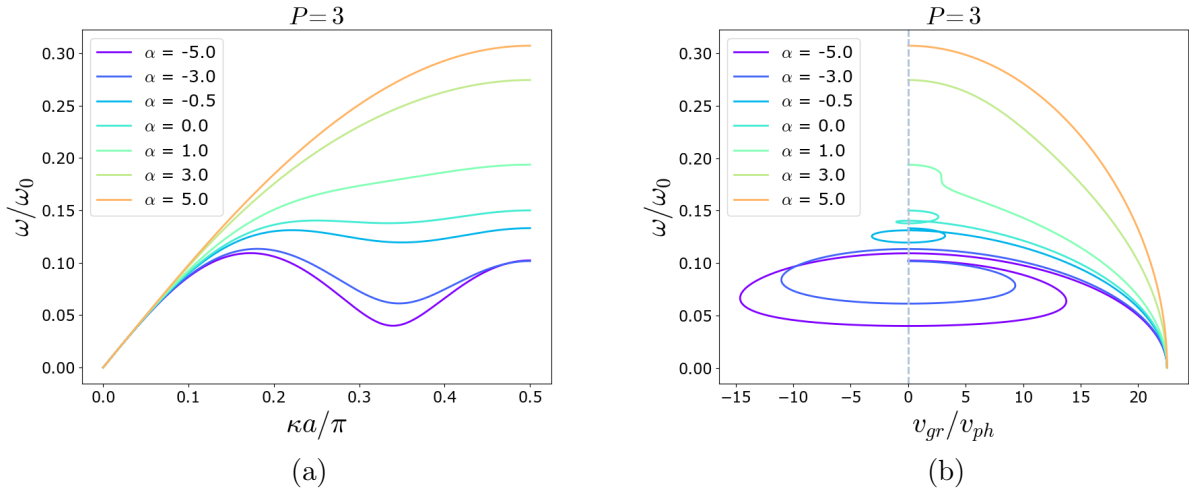


Figure 2.4: Considering a chain with one local and two nonlocal pairings ($P = 3$), in (a) the dispersion curves for different values of α can be observed and in (b) the corresponding group velocities v_g normalised over the phase velocity v_{ph} . The plot entails $\frac{\omega(\kappa)}{\omega_0}$ where ω_0 is v_{ph}/a versus $\frac{v_{gr}}{v_{ph}}$ where v_{gr} is the group velocity over v_{ph} , the phase velocity. The graph in (a) shows the dispersion curves for the chain with $P = 3$ for $\alpha \in [-5, 5]$. Each curve corresponds to a value of α , as stated in the legend. For positive values of α , it can be noticed how the plots appear as classical curves for a discrete local mass-spring chain, while for negative values of α the local minimum corresponding to the roton-like curve in nonlocal chains can be observed. Following the same reasoning, in (b) the vertical line in $\frac{v_{gr}}{v_{ph}}$ separates the positive from the negative values of the group velocity (as the phase velocity is always positive for positive wavenumbers). For negative values of α a larger set of negative $\frac{v_{gr}}{v_{ph}}$ values is attained.

A graphical example of the impact of the two design parameters α and P is described in Figure (2.4) (a) and (b), where the dispersion curves and the group velocity values for a monoatomic chain with a level of nonlocality $P = 3$ are shown for different values of α . Even though the level of nonlocality is fixed, the dynamic behaviour of the chain varies greatly based on how the stiffness is distributed among the links, as it can be observed from the legend, through the assignment of a value of $\alpha \in [-5, 5]$. The chains with negative α values exhibit a roton-like behaviour with a local minimum (Figure (2.4) (a)) and negative group velocity (Figure (2.4) (b)), while the nonlocal chains with stiffness decreasing with nonlocality present a curve similar to that of a local monoatomic chain.

Once the general expressions are obtained, the dispersion curves for different values of α can be derived and the effect on the dynamical behaviour of the chain can be observed, some physically relevant cases emerging from the variation of this stiffness tuning parameter.

In particular, for $\alpha = 0$, it is found from Equation (2.12) that $A_j^{(P)}$ becomes constant and loses its dependency on j , the nonlocality of the spring in question:

$$A_j^{(P)} = \frac{A_1^{(P)}}{j^0} = A_1^{(P)} = A^{(P)} \quad (2.30)$$

In this case it is $A_j^{(P)} = A^{(P)}$ and thus the stiffness of the links results proportional to the inverse of the lengths and to the degree of connection

$$k_j^{(P)} \propto (ja)^{-1} \propto j^{-1} \quad (2.31)$$

hence the stiffness of the link decays as the distance from the connected neighbour increases.

On the other hand, for $\alpha = -1$, $k_j^{(P)}$ becomes constant and can be expressed in analytical form,

$$k_j^{(P)} = \frac{EV_{const}}{a^2 j^0 \sum_{j=1}^P j^2} = \frac{6EV_{const}}{a^2 P(P+1)(2P+1)} \equiv k^{(P)}, \quad \forall P \quad (2.32)$$

This means that every spring has the same stiffness regardless of the enforced degree of nonlocality.

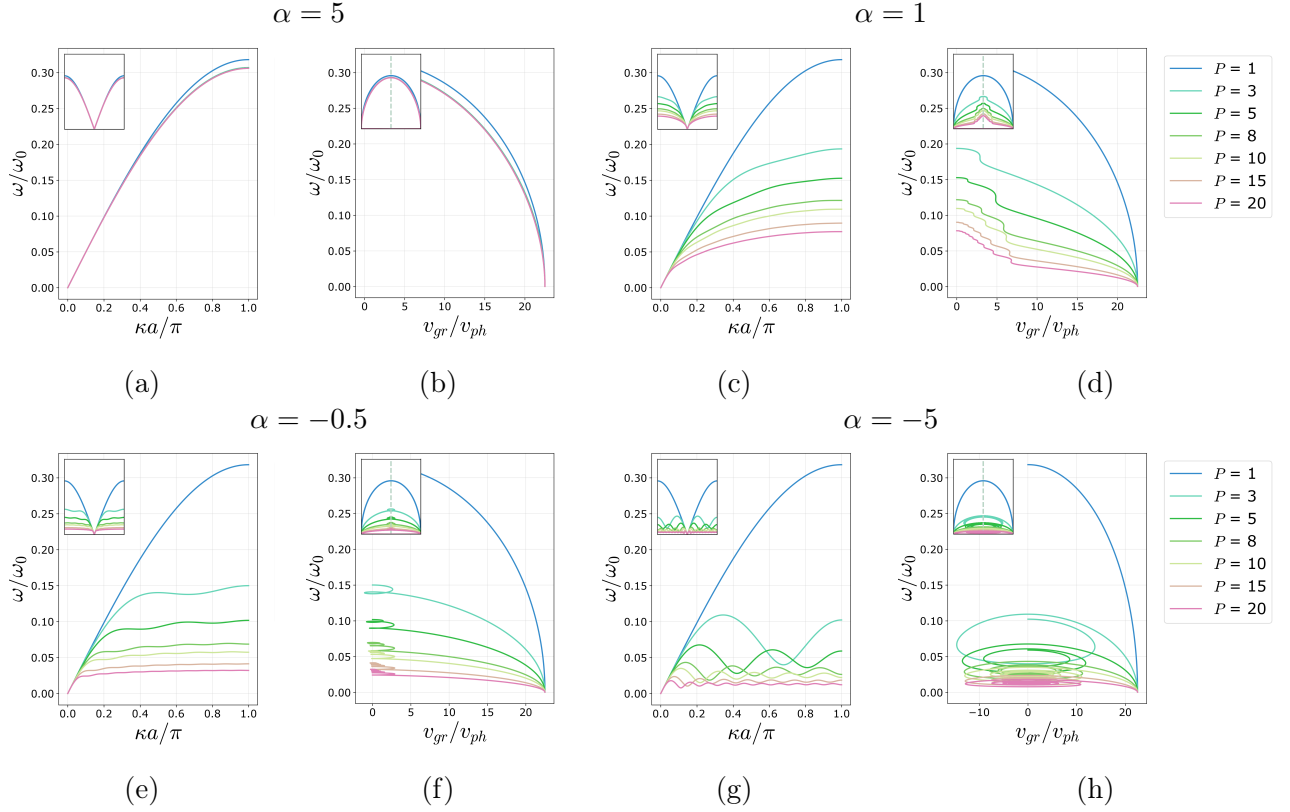


Figure 2.5: In the Figure dispersion relations for irreducible Brillouin zones $\kappa=[0,\pi/a]$ and the corresponding group velocities are shown for different degrees of nonlocal pairings in the monoatomic chain (a), (b) for $\alpha = 5$, (c), (d) for $\alpha = 1$, (e), (f) for $\alpha = -0.5$ and (g), (h) for $\alpha = -5$. It is evident that in the case $\alpha = 5$ the behaviour of the chain is strongly local, be it connected with one spring or many, while for the other limiting case, $\alpha = -5$, several minima and maxima (rotons and maxons) are clearly visible in the curves with $P > 1$ and consequently inversions in the sign of the group over phase velocity ratio can be observed. Noteworthy, in the case $\alpha = -0.5$ the group velocity reaches an inversion in sign, however for a limited amount of values. Finally, in the case $\alpha = 1$, a rather monotonic curve is obtained in every nonlocal scenario, with a non-inverting sign of the group velocity.

Figure (2.5) shows dispersion relations and group velocities for several chains with different degrees of nonlocality P for four significant values of α . As the value of α goes towards higher positive numbers, the behaviour of the monoatomic chain resembles the classical local discrete chain dispersion relation and the frequency increases, as in Figure 2.5 (a) and (b). On the other hand, when $\alpha < -0.5$, the stiffness of the springs connecting BNN masses increases, and the roton-like behaviour of the dispersion relation becomes more consistent, as the local minima in the curve become more evident (and thus the number of wavenumbers corresponding to a negative value of the group velocity increases), as in Figure 2.5 (g) and (h). Figure 2.5 (c), (d), (e) and (f) show the transition for $\alpha = 1$ and $\alpha = -0.5$, and those values are chosen to show how the dispersion curve loses the monotonic behaviour when the stiffness distribution parameter α gears towards negative values.

The frequency shift in the dynamical response is a promising feature, which allows for tuning of the stop bands in and the range of resonance frequencies; in the case of roton-like behaviour the $\omega - \kappa$ relation is in fact not bijective, i.e. more than one κ values correspond to the same value of ω .

The increase in frequency for positive α values is tied to the overall stiffness increase when local links are favoured over nonlocal ones, as the overall stiffness is disadvantaged by the length of the

2.2.7 Time domain simulations and sensitivity analyses

Information on the behaviour of an infinite chain undergoing mass-distribution modifications through changes in the parameter α can be retrieved through its dispersion relation. In this section some insights on the behaviour of a finite mass-spring chain undergoing the same changes will be provided, as to verify that the same kind of dispersion curves can be obtained from a finite model, taking into account some limitations. In fact, nonlocal models require an infinite number of elements in order for the nonlocality level to be attained everywhere. As mentioned in the Introduction, several methods are employed in order to reduce the boundary effects due to the finite nature of numerical and physical models. In this case -discrete- it is necessary for the ratio of the nonlocality level P and the number of masses N to be under a certain threshold, as the bulk of the chain has to weight more than the boundary in the dynamical behaviour. This is needed because the $2P$ boundary masses at the ends of the chain will not satisfy the nonlocality conditions of the considered unit cell, only being connected on one side to their beyond nearest neighbours, and fixed on the other side.

In order to keep the examples within a reasonable computational cost without losing any significant feature of the model nor suffering boundary effects, a 1000 masses chain with fixed ends is thus considered. The chain is excited by means of a harmonic force applied at the center of the chain, with a chirp modulation entailing the resonance frequencies of the system.

The results were obtained from numerical simulations performed in Python through Newmark's method [14]. The initial condition vectors were $\ddot{\mathbf{U}} = 0$, $\dot{\mathbf{U}} = 0$ and $\mathbf{U} = 0$, i.e. no initial acceleration, velocity or displacement were imposed on none of the masses. Mass and stiffness matrices for the finite system $\mathbf{M}, \mathbf{K}$ have been assigned by taking into account the fixed ends. The system was then excited through a time-varying force on the central mass with a chirp modulation in frequency, in order to reconstruct the dispersion curves by acquiring the response to most of the eigenfrequencies of the finite system.

The time-domain results were then processed through a 2D Fast Fourier Transform in order to obtain the results in the frequency domain, i.e. the dispersion curves for the finite chain. The results can be observed in Figure 2.6, where the numerical dispersion curves for mass-spring chains with levels of nonlocality $P = 1, 5, 10$ and stiffness distribution parameter $\alpha = -5, -0.5, 5$ are shown. The attained curves confirm the results predicted analytically for the infinite periodic chain, confirming the hypothesis that for a low enough ratio between the number of masses N and the level of nonlocality P the boundaries do not interfere with the dynamical behaviour of the bulk of the chain. It can be observed how in Figure 2.6 (a), (b) and (c) the dispersion relations resemble the classical curves of a monoatomic local chain, regardless of the level of nonlocality P , due to the positive value of the stiffness distribution parameter α . However, when the value of α reaches negative values, as in Figure 2.6 (d),(e),(f),(g),(h) and (i), the roton-like effects can be retrieved, with the local minima and maxima being proportional to the level of nonlocality of the chain.

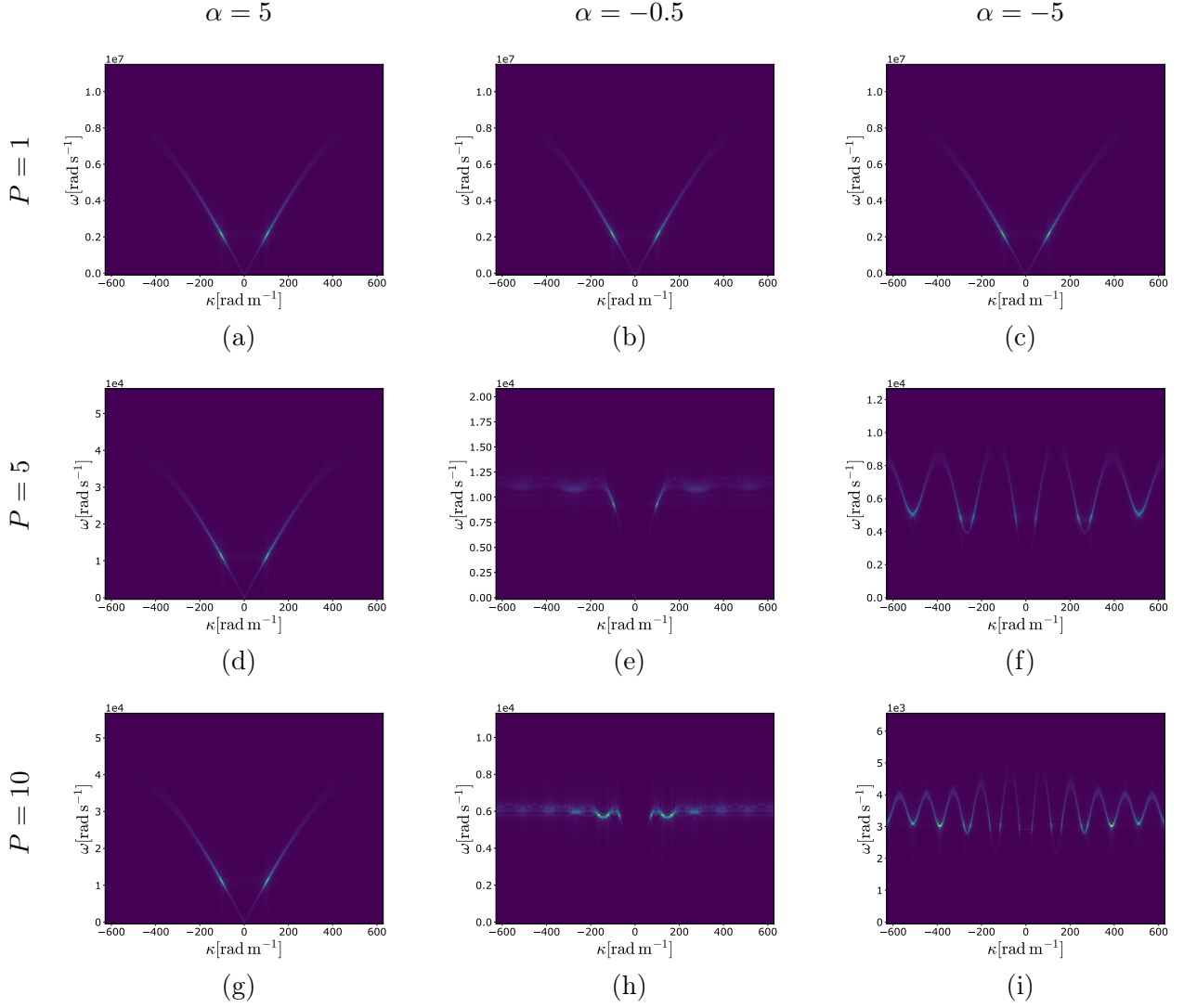


Figure 2.6: In this figure the $A(\kappa, \omega)$ contour plots for 2D FFTs of the time-domain simulations are shown, where the amplitude A of the frequency response increases with the contrast between the dispersion curves and the background, and depends on the excitation. In the graphs, the frequency ω in rad/s and the wavenumber κ in rad/m spanning the first Brillouin zone are respectively on the ordinate and abscissa axes. The chain is constrained at both ends, the masses being equal, with $m = 1\text{kg}$, and the constants $E = 500\text{GPa}$, $V = 1\text{m}^3$, $a = l_0 = 0.005\text{m}$. Input parameters entailed 1000 masses, level of nonlocality $P \in [1, 10]$, input force $F = F_0 \cos(\omega(t)t)$, where $F_0 = 1\text{N}$ and forcing frequency ω varying at each time step through a chirp modulation, in the range of the natural frequencies of the chain. The images illustrate the propagation behaviour for different P and α values, as indicated explicitly on the left and top sides. Note that, despite growing levels of nonlocality, when the value of α is positive no significant changes in the dispersion curves appear, as predicted by the theoretical model. On the contrary for negative values of α the curves lose the monotonic behaviour and exhibit a number of local minima proportional to the nonlocality level.

2.3 Results and Discussion

In this work, a mass-conservation law for the springs in a nonlocal monoatomic chain was conceived. Two parameters were then introduced, the nonlocality level P and the stiffness distribution α , with

the aim of allowing for tuneability in the models. The impact of the parameter α on how the mass and proportionally the stiffness distributes among the local and nonlocal pairings is summarised in the illustrations in Figure 2.7, where in (a) and (b) α assumes respectively a positive and negative value.

Analytical predictions were made through infinite models, following Bloch-Floquet and Brillouin's theories, and the role of the nonlocality level P and the stiffness distribution parameter α in obtaining roton-like curves was highlighted. The obtained results were then validated through numerical simulations on a finite chain, which confirmed the analytical predictions.

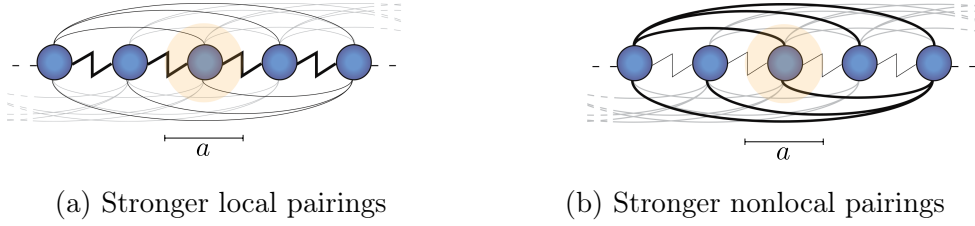


Figure 2.7: Comparison of local and nonlocal pairings with a positive (a) and negative (b) value of the stiffness distribution parameter α

Two main, equally relevant reasons motivated the choice of forcing the springs masses to be constant. One is a matter of mechanical consistency, which is believed to be required for any mono-atomic chain model comprising an arbitrary number of elastic links. In fact, when mass-spring models are employed to simulate dynamical systems, only masses are considered as contributors to the inertia and to the natural frequency of the structure. The usually local springs have negligible mass compared to that of the oscillating masses. However, as the nonlocal connections increase and the mass of the physical links increases accordingly, its contribution might become relevant to the dynamics, making this kind of model progressively less accurate as the level of nonlocality (say the number of links) increases. In the limit of a "fully nonlocal" chain made of infinite masses (i.e. all the atoms are linked to each other), one would fall into the paradoxical situation of divergent total spring masses and the hypothesis of negligible mass of the links with respect to the mass of the atoms would be evidently violated. On the contrary, by imposing *a priori* a constraint on the total mass of the springs, the difference in the order of magnitude between the masses of the beads and of the connections would be automatically preserved, and thus the validity of the model. It is worth to highlight that forcing the springs mass to be constant is not a constraint to be reserved for 1D nonlocal chain models, since the same line of reasoning holds true for 2D and 3D lattices. Additionally, a note on nonlocal continua is perhaps due. In fact, for nonlocal continuous media (e.g. integral nonlocal elasticity, peridynamics, and other models) the stiffness is modulated through the variation of the Young moduli with the distance between each pair of material points: as a consequence, at least in absence of underlying hypotheses about the micro-structure, nonlocality only depends on the intrinsic elasticity of the ground material and thus does not involve additional masses to be somehow balanced. The second reason for which it is felt that the conservation of springs mass must be considered as a necessary constraint to nonlocal model is related to a matter of engineering/physical rationality. In fact, it is well known that any problem in the structural mechanics context, be it static or dynamic, aimed at finding a design optimum, needs an object function and a constraint, the former furnishing the measure of the advantage one would gain in making a choice and the latter being exactly the parameter with respect to which one can compare two or more models. In Mechanics, for instance, design optimization of the shape of structures or topology optimization of materials are performed under prescribed boundary conditions and materials, selecting an object function (e.g. maximum stiffness) and imposing a constraint (e.g. the total mass of the element). In this way, two possible choices can be discriminated –and

two models compared– by evaluating, among all the possible configurations (sizes of cross sections in structurally optimized beams or spatially non-homogeneous density distribution in topologically optimized materials) the one(s) giving the best needed performance, but under the given constraint (typically prescribing the total amount of available mass).

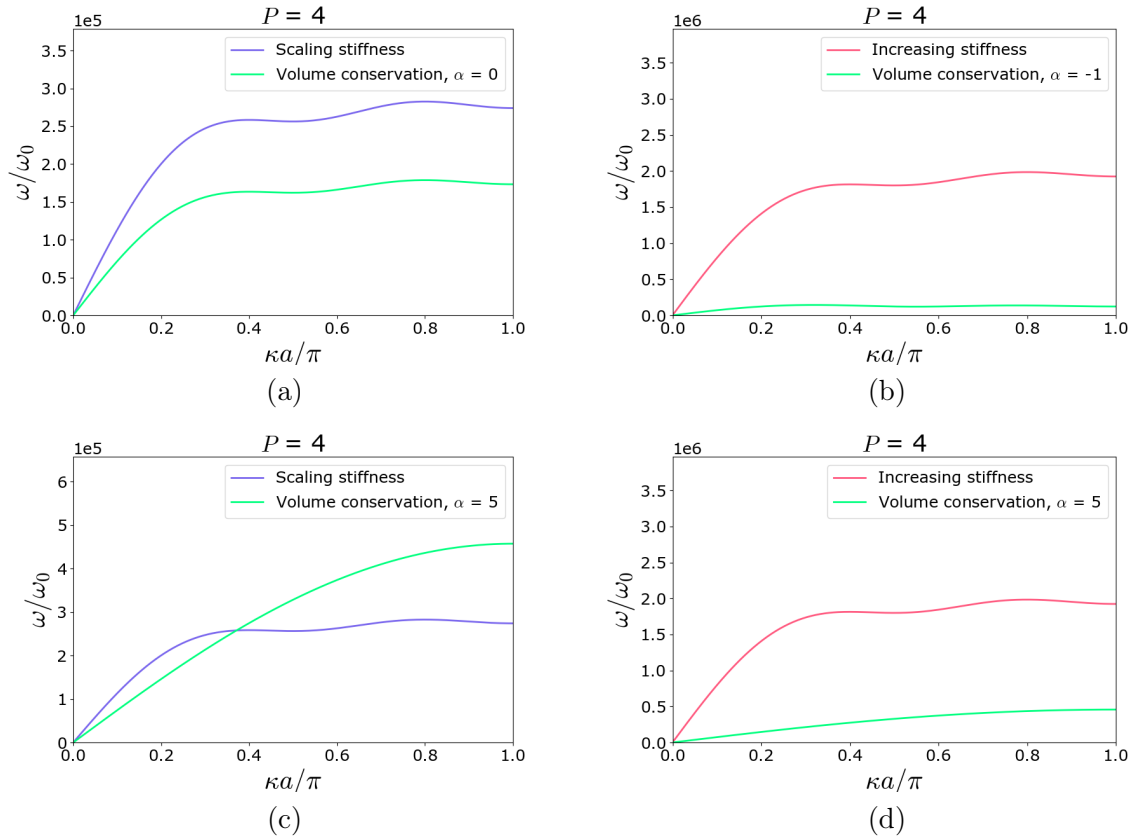


Figure 2.8: Comparison between the proposed volume-conservation model (in green), a model with stiffness scaling (decreasing) with distance (in blue, (a) and (c)) and a model with constant stiffness regardless of the level of nonlocality, thus overall increasing with the number of pairings (in red, (b) and (d)), all three with a level of nonlocality $P = 4$. In (a) it can be noticed that for a chosen value of the α parameter a similar behaviour to the curve of the non-parametric model (in blue) can be obtained, as a similar scaling is attained in the volume-conserving case while retaining the mechanical constraint. The curve corresponding to our model (in green) features a lower frequency range as the overall stiffness is affected by the volume conservation. The advantages of adopting a power law with a further degree of freedom in designing the nonlocal chain, given by α , are pointed out in (c), as by the sole tuning of the parameter the frequencies can be increased without switching to another scaling law. In (b) and (d), different behaviours retrieved by variation of α are compared to the fixed, non-tuneable, increasing stiffness model. The volume-preserving model allows for changes in the dispersion relation according to the selected α value within a small frequency range.

Concerning the applicability of the principle, some limitations need to be mentioned, as it is a theoretical 1D model that describes a phenomenon to its bare main features. The applications to higher order models in 2D or 3D, for waves with transverse or composed components would require further study and taking into account more factors, as the overall geometry, local resonances or the axes for roton-like propagation. However, it is felt that even the limited information a 1D model can give are crucial to the understanding of complex phenomena, when the simplification does not rule out

important factors from the physics of the problem. A further limitation is in the number of nonlocal neighbours that can be connected in a finite model. In fact, when considering an infinite mass-spring chain, any number P of beyond nearest neighbour connections can be taken into account. On the other hand, when considering a finite model with N masses, the ends of the chains will be connected only on the left or on the right to the rest of the chain, thus supporting $N - P$ nonlocal connections. The level of nonlocality for which border effects can be ignored in the overall dynamical behaviour is thus proportional to the number of unit cells present in the designed model. Nevertheless, the study of the effects of the boundary conditions on the dynamics of nonlocal monoatomic chains would deserve a deeper reflection to analyse with due attention their theoretical and physical implications, including sensitivity analyses in order to quantify the boundary influence over the behaviour of the bulk of the periodic system, which are beyond the purpose of the present work.

Some advantages for design purposes of the approach presented in this study are instead highlighted here. The volume, i.e. mass, conserving approach is tested in comparison to hypothetical scaling laws that one could employ to scale stiffness at different levels of nonlocality and analyse nonlocal behaviour in mass-spring chains, which do not involve any mechanical consistency condition. In Figure 2.8 some example dispersion relations are shown, with a direct comparison between the proposed model (in green) and two other models. The first of these models, shown in blue, is characterised by a stiffness with a scaling law in the form

$$k_j^{(P)} = \frac{k_1^{(P)}}{j}, \quad j \in \{1, \dots, P\} \quad (2.33)$$

where

$$k_1^{(P)} = \frac{EA_0}{a} \quad (2.34)$$

with A_0 and E constant. The stiffness is thus linearly decreasing with nonlocality.

The second of these models, shown in red in the graphs, simply features the same stiffness for every spring added to the system, as

$$k_j^{(P)} = k^{(P)} = C, \quad \forall j \in \{1, \dots, P\} \quad (2.35)$$

with C being a given constant value, thus leading to an overall stiffening of the chain with the increase of nonlocal pairings and to a consequent rise in frequency. In the volume conservation hypothesis, the stiffness of each spring is constant in the case $\alpha = -1$, however the total volume (mass) remains constant and abides by the *mechanical consistency condition*.

It must be also pointed out that the model here proposed allows a larger degree of freedom in tuning the dynamic behaviour of a chain made by a fixed amount of material. By tuning the stiffness distribution parameter α , it appears clear how the proposed mass conservation law not only ensures mechanical consistency, but also allows to span through multiple frequency ranges and behaviours that would need to be otherwise *a priori* fixed by the choice of a certain scaling law over another.

2.4 Conclusions and perspectives

Overall, the present proposal stems from the necessity and convenience of establishing a rule based on a clear physical meaning to determine the relationship between the degree of nonlocality and the stiffness of the connections between the particles. The mass conservation is key here, not only for ensuring mechanical consistency of the models, but also to allow fruitful dynamical comparisons between designs characterised by different parameter values. From a theoretical point of view, as stressed above, it is important for considering the springs massless in the mass-spring model that the dynamics are not influenced by the springs' mass. The practical value of the principle answers to the need to

compare different models for establishing the optimal level of nonlocality and the way in which spring stiffnesses vary with the distance of the connected masses, with respect to an object function. Moreover it is important for consistency of the comparisons between different dynamical models. As for further developments, an experimental validation of the proposed model could be envisaged. In Figure (2.9) the scheme of a possible geometry is represented. Eventually it would subsequently be possible to design mass conservative unit cells in more than one dimension and manufacture the prototypes with 3D printing machines. However, as previously cited, it would entail more steps in the design process as choosing the kind of elastic waves, the most appropriate direction for the roton-like propagation in the imagined model and the possible interference given by local resonances.

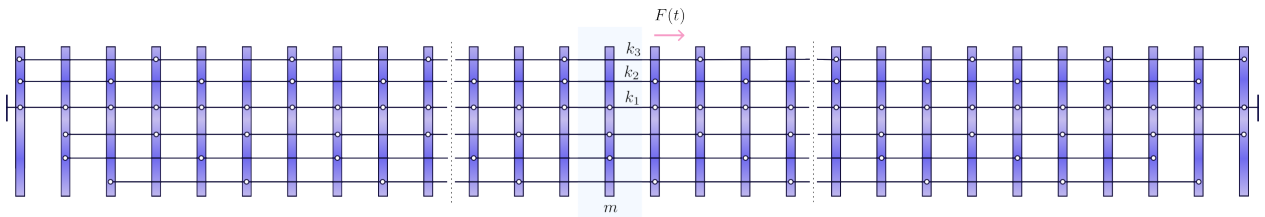


Figure 2.9: Possible scheme of a reduced and simplified experimental model, with fixed ends. The element marked by m is unit mass while the linear elements connecting them at different levels of nonlocality are the linear elastic springs. The model is possibly hanged on a support, and free at both ends, so that the waves can completely reflect (or alternatively fixed at both ends to achieve the same effect). The number of unit cells present in the model should be enough to obtain a sufficient number of points in the space reciprocal to the coordinates space (x), that is the wavenumber space (κ). The model should be fixed in order to limit the transverse modes as much as possible, as the first validation should be for a one-dimensional model as the imagined one. The dynamic excitation $F(t)$ could be carried out by a waveform generator coupled with a piezoelectric patch on one end of the chain. The input signal would be designed through an iterative procedure in order to obtain the optimal frequencies, as it is necessary to excite as many natural frequencies as possible in order to construct the dispersion curves accurately. Furthermore exciting higher frequencies could represent a challenge both in the exciting force and the retrieving of the displacement data. However, as in the case of the numerical simulation, the idea for the input signal would entail a chirp signal with frequencies $f = \omega_i/(2\pi)$, with $\omega_i \in \Omega = [0, \omega_N]$, where Ω is the set of the N eigenfrequencies of the N masses of the prototype ($N \approx 100$), that could be analytically or numerically estimated. The displacement amplitude $u(x, t)$ for each mass could be subsequently retrieved for example by using high-speed cameras, subtracting the initial positions. The resulting data with an error estimate would then be treated by a Fourier transform to obtain the experimental dispersion curves.

Naturally, this line of reasoning can be easily extended to encompass more complex models, which may feature different interactions between masses, such as shear ones. For instance, the proposed conservation model would still apply in considering a classical shear stiffness of the type

$$k_j^{(P)} = \frac{GA_j^{(P)}}{\chi pa} \quad (2.36)$$

where G is the shear modulus and χ the shear factor. If we were to consider bending stiffness or torsional stiffness, the expressions would instead read

$$\begin{aligned} k_j^{(P)} &= \frac{12EI}{(ja)^3} \quad \text{for bending} \\ k_j^{(P)} &= \frac{GI_p}{ja} \quad \text{for torsion} \end{aligned} \tag{2.37}$$

where in the case of bending a clamped configuration at both ends is considered. In these cases the scaling on the cross section $A_j^{(P)}$ is included in the inertia of the section, that could be considered for instance square with $I = \frac{A_j^{(P)2}}{12}$, or circular with $I_p = \frac{A_j^{(P)2}}{4\pi^2}$.

It is thus felt that the proposed mass conservation condition and the suggested criteria for guiding the transition from local to nonlocal monoatomic chains may help to conceive new classes of metamaterials and to design and realize 3D prototypes, based for instance on advanced additive manufacturing processes.

Chapter 3

Diatomic nonlocal one-dimensional chains from mass-shift induced defects

Abstract

Mechanical metamaterials and wave-filtering devices have proven their potential in controlling wave-propagation through the tailoring of their dispersion curves, i.e. the relation between wavenumbers and frequencies, to specific engineering needs, allowing for blocking, filtering or focusing the incoming noise and vibration. Their properties rely on their periodic lattice structure, made out of one or multi dimensional arrays of unit cells, interacting with one another. Taking into account beyond-nearest-neighbour (BNN) connections, i.e. interactions between non-neighbouring unit cells, has given metamaterial design a new perspective, thanks to their peculiar roton-like dispersion curves, with local minima and maxima corresponding to inversion in the wave (energy) propagation direction. The manufacturing of wave-filtering devices still poses, however, multiple challenges, which include accounting for imperfections. In fact, defects can significantly alter the behaviour of these systems, making the study of their impacts both necessary and interesting. Nonlocal interactions can intensify or mitigate the effects of impurities, for instance by hindering the blocking effects of a band-gap or broadening one. This work builds on a previous study by the present authors on monoatomic nonlocal chains, where a mechanical consistency condition was established in order to ensure a physically sound mathematical simulation process and enable comparisons between different prototypes. A mass-conserving model is considered, with a fixed small ratio between the mass of the springs and of the atoms, as in nonlocal models the masses of the links could become relevant in the system dynamics, while it is usually neglected in mass-spring chains. An odd mass distribution between elements of the same kind (masses or springs) can take place, through *mass shifts* in two consecutive unit cells. In this context, a diatomic configuration is derived. The dispersion relation contains two branches, the acoustical and the optical one, which are impacted in position and shape both by the mass distribution between the defected elements and by the parameters governing the model, the stiffness distribution α and the nonlocality level P . The dispersion curves are analytically derived in function the parameters cited above, and the transition between a diatomic and a monoatomic chain are highlighted. Finally numerical studies on finite chains confirm the analytical predictions on infinite ones, and a brief discussion on localised imperfections is carried out. The hereby proposed approach supplies a framework for designing metamaterial and wave-filtering devices which account for -or even exploit- imperfections, adding further insights into developing robust prototypes.

3.1 Introduction

This Chapter builds on the concept of nonlocal one-dimensional mass-spring systems, described in Chapters 1 and 2.

3.1.1 Defects and imperfections

As metamaterial and/or periodicity based devices rely on the design of their unit cells to attain certain dynamic behaviours, the prototypes are often intricate and detailed, and their manufacturing is no easy task. Some of the possible manufacturing processes involve laser cutting or 3D printing. As the periodicity plays an essential part in the functioning of such devices, the almost exact resemblance of one unit cell to another is fundamental to obtain the desired results. Industrial processes involve however certain error allowances that cause the lattices to have small defects or imperfections. These can be almost repeated (leading to quasiperodicity) or localised to a certain area of the lattice, with different impact on the envisaged design and perturbation of the outcomes of the analysis of the perfect lattice. In solid state physics, the effect of defects in crystals and periodic structures has been investigated thoroughly, leading to the formulation of *Anderson localisation* [72]. In fact, in some conditions a defected unit cell - in geometry or material properties - can lead to energy dissipation outside its boundaries, i.e., localisation of vibration in a single point. In the metamaterial field this is also known as a localised mode, with an almost constant frequency value for the whole wavenumber span. Depending on the characteristics of the lattice and of the imperfection, this can lead to excited frequency above the traditional band stop of the unperturbed material, or to a localised mode inside of a bandgap, where usually wave propagation would not happen.

3.1.2 Energy harvesting

The energy localisation properties could help develop some energy harvesting devices, e.g. for self recharging small items as controllers and sensors, by exploiting vibrational energy already dispersed into the environment instead of using electrical batteries, reducing the need for raw materials and mining, and increasing environmental compatibility. The opportunities offered by ad hoc defected lattices for energy harvesting have been investigated in the metamaterial field for several kind of waves, following the same principles. Carrara et al. [73] focus on harvesting energy for small devices through elastoacoustic waves, whose energy is transduced to electrical through piezoelectric patches. They propose a parabolic acoustic mirror that allows for uncertainty in the point source of vibration, while retaining the capacity for energy enhancement and conversion. Conversely, Chaplain et al. [74] exploited the rainbow effects in waveguiding for energy harvesting purposes, by creating lattices to trap, focus and convert energy. These devices exploit dispersive properties which lead to zero group velocity (ZGV) modes, that lead to energy not propagating neither forward nor backwards in the lattice. These modes are analysed in their work, and a distinction is made between ZGV modes that do indeed trap energy and avoid its propagation and ones that do consent it after an initial delay. Another approach, put in place by Oudich et al. [75], involved working on energy harvesting in the acoustic field through the design of metamaterial plates. Their work exploited the local resonance phenomenon, by adding mass-spring resonators into the lattice. The analysis embraces both the dispersion properties and the mechanical-to-electrical energy transduction process. Concepts borrowed from topological analysis of unit cells and their interfaces provide further tools for the localisation of energy. Pal et al. [76] delved into the relationship between topological properties of lattices and their effect on wave localisation. It is shown that some localised modes can start at the boundaries and travel to the bulk of the material, through appropriate parameter choices. In [77], Zalipaev et al. study the case of defects in junctions of thin walled bridges, where localised eigenmodes due to the defect emerge. It is proven that standing waves appear in lattices with periodic defects.

3.1.3 Topology, localization and waveguiding

Topological properties do however provide a wide spectrum of possibilities for wave manipulation purposes. In fact, another major leap forward in metamaterial design in the last decade was the discovery of the impact of crystal symmetries on the topological properties of materials with applications in a broad set of fields, from electromagnetism ([45], [78]) to acoustics ([79], [80] [81]) to mechanics. Non-trivial symmetries let researchers achieve promising features as waveguiding without backscattering loss and vibration and sound isolation. The topological understanding of the behaviour of periodic system allows the design of specific boundary conditions and band structures for waveguiding ([82] or localization [76], which are unimpaired by the presence of fabrication defects and impurities, thus yielding reliable devices. [83] Guiding the waves along a specific path without being scattered or reflected back is of crucial importance for a more efficient transmission of energy. [84]

Band structures with a topological nature are characterised by a topological invariant [85]. This concept arises from an analogy with a quantum phenomenon arising in electronic structures, the quantum Hall effect ([86],[87]), whose topological aspects are described by the Chern number, calculated by integrating the Berry curvature over the Brillouin zone, or the winding number, corresponding to the Zak phase ([88],[89]). The nontriviality of topological invariants indicate the presence of different states with different propagation properties. The symmetries involved in topological characterisation of materials are distinct, such as time-reversal symmetry, particle-hole symmetry or chiral symmetry [90].

The variation of the topological properties of a lattice can be obtained through the breakage of the symmetry and periodicity, namely by integrating defects in the structure [91]. These can be introduced in a system through altering its periodicity both in geometric and material parameters in a specific region. Defects can be point, line, planar or bulk [92] and their influence on wave propagation has been studied in different configurations in a mass-spring lattice ([93],[94]). In [95] it is shown that smaller masses or higher stiffness in the springs of a mass-spring chain lead to localised modes. Depending on the kind of impurity, several different wave behaviours can take place.

Along with the waveguiding, wave localization, as mentioned earlier, is another meaningful aspect that arises due to topological implications.

Localization of waves is a phenomenon in which a wave, e.g. eletro-magnetic or elastic, is trapped or localized in a disordered medium, leading to the absence of diffusion. It is also known as Anderson localization ([72], [96],[97],[98], [99],[100]) after P.W. Anderson, who first observed the localization behaviour due to defects or impurities.

In theoretical physics [101] Hasan and Kane have provided a thorough foundation for topological considerations in material models. They provide a essential groundwork on topological insulators and superconductors in 1D, 2D and 3D.

A extensive study on the topic and its applications to metamaterials was carried out by Suesstrunk and Huber [102], who write from a solid state physics background. The goal of this work is to bridge the gap of the topological classification of phonons in electronic systems and mechanical ones, with the end goal of easing the application of these ideas to metamaterials. They provide an overview of the symmetry classes and their effect on wave propagation.

A recent review by Miniaci and Pal [103] focuses on the technical steps needed to design waveguiding devices through topological concepts, which involve geometric and symmetry properties. In the elastic waves domain this approach could give a groundbreaking contribution due to the fact that different polarizations of elastic waves often hybridise and it is consequently very complex to isolate a polarization. The paper provides a framework to work with these concepts.

In photonics topological properties enable the realisation of opto-acoustical cavities and backscattering protected metamaterials ([104],[105])

Examples of designs from the phononic crystals and metamaterial community include metamaterials with low frequency modes ([106], [107]), gyroscopic devices that prevent backscattering [108],

localization of flexural waves [109], and even applications in statics [110]. In mechanical metamaterials experimental proof of these concepts is given by Li and coworkers [111].

For one-dimensional mass-spring chains the archetypical model to take into consideration as simplest topological model is the Su-Schrieffer-Heeger (SSH) model [112]. The SSH model is a one-dimensional mass-spring chain that presents a biatomic periodic unit cell characterized by two identical masses and two different springs, as representative of a dimeric chain with single and double bonds. It has been shown that in this model the variation in the spring stiffness ratio causes band inversion through gap closure, and two different topological phases before and after. When two chains which are periodic in opposite directions with two different topological phases are bound together, a localization phenomenon arises, that causes wave trapping in the case of the one-dimensional chain [113] and provides a waveguide in two- or three-dimensional geometries. This is due to the bulk edge correspondence [87]. Extensions of this model have allowed more research based on mass-spring lattices, useful in continuum approximations ([114], [115]).

The correlations between nonlocality and defects have drawn the attention of some authors, however they have yet to be completely unveiled. In a paper from 2000 [116], Hennig has explored the connection between these phenomena in the quantum domain, displaying how next nearest interactions enhance localized soliton-like solutions in polymer chains modelled with the nonlinear Schroedinger equation. In 2018, Perez et al. [117] have studied the topological behaviour of the SSH model when extended to nonlocal systems, (i.e. with long range interactions). As highlighted in their paper, BNN interactions can produce both topological triviality and larger topological invariants (Zak phase, winding numbers, that are limited to two values, 1 and 0, in the classical SSH model) depending on which symmetries are preserved in the model chain through even or odd hoppings, in which case even more edge states could be obtained. By introducing disorder in the lattice, these authors have shown that off-diagonal disorder affects edge states in both the classical and extended SSH chain. Chen et al. exploit the long range pairings in SSH models to test the endurance of chiral symmetries under deformations [118]. De Moura et al. [119] studied the correlations between nonlocality, localization and disorder. They examine collective excitation in a chain of nonlocally connected masses and the energy bands for different wave numbers, thus discovering that energy transport can be strongly influenced by long range interactions and randomness of the masses.

In this Chapter the impact of beyond nearest neighbours, i.e. nonlocal, interactions in mass-conserving lattices with imperfections is studied. The starting point of the analysis is the monoatomic chain model discussed in Chapter 2, where the mass conservation law is first established. In this Chapter, some imperfections that could arise from manufacturing are enforced on the one-dimensional lattice. The imperfections are first considered to arise from a shift in the mass distribution in the springs, in the atoms, or both, so that a diatomic configuration with the overall amount of material unchanged is retrieved. Secondly, the impact of the mass shifts is combined to a localised imperfection in a numerical analysis, and the defect modes that appear are observed.

With a focus on the established parametric conservation law that rules over the behaviour of the chain, by varying the stiffnesses and the number of the springs involved, the analysis means to observe the gradual impact of the nonlocality and the strength of the pairings on the behaviour of configurations that lose the monoatomic periodicity and involve more than one mass in the unit cell instead.

3.2 Methods and analysis

In this section, the theoretical framework and the analytical analyses are carried out on infinite, periodic one-dimensional lattices.

3.2.1 Perturbation of the monoatomic, periodic mass-spring chain

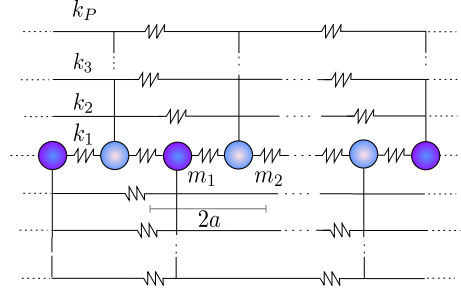


Figure 3.1: P level BNN connected diatomic chain, with $2a$ unit cell length.

The first step to this analysis, involves considering the case in which the mass distribution between two subsequent masses is not equal. This means, from a definite amount of mass m assigned theoretically to each mass, the masses m_1 and m_2 of two masses in two sequential unit cells will be

$$m_1 = m + \Delta m, \quad m_2 = m - \Delta m \quad (3.1)$$

with

$$m > 0, \quad \Delta m > 0, \quad m > \Delta m \quad (3.2)$$

thus

$$\begin{aligned} m_1 &= m + \Delta m > 0 \\ m_2 &= m - \Delta m > 0, \end{aligned} \quad (3.3)$$

This is the first imperfection considered in the lattice, which at the limit $\Delta m \rightarrow 0$ coincides with the monoatomic configuration. If the shift in distribution only concerns two unit cells next to each other, a diatomic model arises from the defective configuration.

The same reasoning can be applied to the mass-conserving springs which link the local and nonlocal elements of the chain, by considering for the same level of nonlocality $j \in [1, P] \subseteq \mathbb{N}$, $P \in [1, +\infty[\subseteq \mathbb{N}$,

$$k_{j,1}^{(P)} = k_j^{(P)} + \Delta k_j^{(P)}, \quad k_{j,2}^{(P)} = k_j^{(P)} - \Delta k_j^{(P)} \quad (3.4)$$

where $k_{j,1}^{(P)}$ and $k_{j,2}^{(P)}$ are considered to connect the mass they radiate from respectively to its local or nonlocal neighbour to the left and to the right.

3.2.2 Diatomic chains with odd atom masses

When a shift in the mass distribution among the beads is considered, as in the definitions in equation 3.1, the motion of the nonlocal diatomic unit cell can be described as a system of two equations as follows

$$\begin{aligned} m_1 \ddot{x}_{2n} &= \sum_{j=1}^P k_j^{(P)} (x_{2n+j} + x_{2n-j} - x_{2n}) \\ m_2 \ddot{x}_{2n+1} &= \sum_{j=1}^P k_j^{(P)} (x_{2n+1+j} + x_{2n+1-j} - 2x_{2n+1}) \end{aligned} \quad (3.5)$$

where for even and odd values of j the masses are connected respectively to masses with positions multiples of $2n, 2n + 1$ respectively in the lattice.

The wave solution is assumed to take the following form

$$x_{2n} = \Omega_1 e^{i(\kappa 2na - \omega t)} \quad (3.6)$$

$$x_{2n+1} = \Omega_2 e^{i(\kappa(2n+1)a - \omega t)} \quad (3.7)$$

where Ω_1, Ω_2 represent the wave amplitudes and a is the lattice unit length.

Substituting the solution into the system and considering the Bloch-Floquet periodic boundary conditions, the equations of motion become

$$-\omega^2 \Omega_1 m_1 = \sum_{j=1}^P k_j^{(P)} \times \begin{cases} \Omega_2 e^{i\kappa ja} + \Omega_2 e^{-i\kappa ja} - 2\Omega_1 & \text{if } j \text{ odd} \\ \Omega_1 e^{i\kappa ja} + \Omega_1 e^{-i\kappa ja} - 2\Omega_1 & \text{if } j \text{ even} \end{cases} \quad (3.8)$$

$$-\omega^2 \Omega_2 m_2 = \sum_{j=1}^P k_j^{(P)} \times \begin{cases} \Omega_1 e^{i\kappa(j)a} + \Omega_1 e^{i\kappa(-j)a} - 2\Omega_2 & \text{if } j \text{ odd} \\ \Omega_2 e^{i\kappa(j)a} + \Omega_2 e^{i\kappa(2-j)a} - 2\Omega_2 & \text{if } j \text{ even,} \end{cases}$$

where the solutions for even and odd values of $j \in P$ have been separated. In fact, in the nonlocal lattice the connection can happen either between two different masses $m_l, m_m, l \neq m$, whose periodic solution will differ in amplitude $\Omega_l \neq \Omega_m$, or between beads with masses $m_l, m_m, l = m$, whose solution will have the same amplitude value $\Omega_l = \Omega_m$.

Remembering that $m_1 = m + \Delta m$ and $m_2 = m - \Delta m$, the dispersion curves can be written as

$$\bar{\omega} = -\left(\frac{2m}{m^2 - \Delta m^2}\right) \Delta C \pm \sqrt{\left(\left(\frac{m}{m^2 - \Delta m^2}\right) \Delta C\right)^2 - \frac{1}{m^2 - \Delta m^2} (C_1^2 + C_2^2 - 4C_3^2 - 8C_1 C_2)} \quad (3.9)$$

where $\Delta C = C_2 - C_1$, and, from the definition of $k_j^{(P)}$ in equation 2.14, the coefficients of the eigenvalue equation can be rewritten as

$$C_1 = \sum_{j=1}^P 2 \frac{EV_{const}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} \quad (3.10)$$

$$C_2 = \sum_{j=2}^{P_{even}} 2 \frac{EV_{const}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} (\cos(j\kappa a)) \quad (3.11)$$

$$C_3 = \sum_{j=1}^{P_{odd}} 2 \frac{EV_{const}}{a^2(j^{1+\alpha})} (\cos(j\kappa a)) \quad (3.12)$$

For a complete derivation of the analytical results, see A.1.

3.2.3 Diatomic chains with odd spring masses

The second case of defective mass-conserving chain, a shift in the distribution of the spring's mass is considered. Therefore,

$$\begin{aligned} k_{a,j}^{(P)} &= k_j^{(P)} + \Delta k_j^{(P)}, \quad j \in 1, 2 \dots P \\ k_{b,j}^{(P)} &= k_j^{(P)} - \Delta k_j^{(P)}, \quad j \in 1, 2 \dots P \end{aligned} \quad (3.13)$$

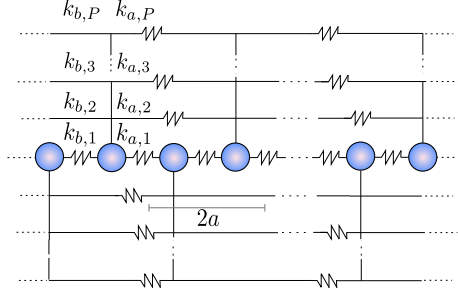


Figure 3.2: P level BNN connected diatomic chain, with $2a$ length of the unit cell.

where the stiffness value is shifted on the springs of each nonlocality level. Equations are subject, as in the previous case, to the following conditions for the *mechanical consistency* condition to be valid,

$$k_j^{(P)} > 0, \quad \Delta k_j^{(P)} > 0, \quad k_j^{(P)} > \Delta k_j^{(P)} \quad (3.14)$$

thus

$$\begin{aligned} k_{a,j}^{(P)} &= k_j^{(P)} + \Delta k_j^{(P)} > 0 \\ k_{b,j}^{(P)} &= k_j^{(P)} - \Delta k_j^{(P)} > 0, \end{aligned} \quad (3.15)$$

The configuration of the chain thus turns once again from monoatomic to diatomic, as for every second mass the connections' stiffness on the right and on the left handside is inverted. The equations of motion read

$$\begin{aligned} m_1 \ddot{x}_{2n} &= \sum_{j=1}^P k_{a,j}^{(P)} (x_{2n+j} - x_{2n}) + \sum_{j=1}^P k_{b,j}^{(P)} (x_{2n-j} - x_{2n}) \\ m_2 \ddot{x}_{2n+1} &= \sum_{j=1}^P k_{a,j}^{(P)} (x_{2n+1+j} - x_{2n+1}) + \sum_{j=1}^P k_{b,j}^{(P)} (x_{2n+1-j} - x_{2n+1}) \end{aligned} \quad (3.16)$$

As in the previous case, the two solutions are 3.6 and 3.7. Plugging them into the system yields

$$\begin{aligned} -\omega^2 \Omega_1 m &= \sum_{j=1}^P k_{a,j}^{(P)} \times \begin{cases} \Omega_2 e^{i\kappa j a} - \Omega_1 & j \text{ odd}, \\ \Omega_1 e^{i\kappa j a} - \Omega_1 & j \text{ even}, \end{cases} + \sum_{j=1}^P k_{b,j}^{(P)} \times \begin{cases} \Omega_2 e^{-i\kappa j a} - \Omega_1 & j \text{ odd}, \\ \Omega_1 e^{-i\kappa j a} - \Omega_1 & j \text{ even}, \end{cases} \\ -\omega^2 \Omega_2 m &= \sum_{j=1}^P k_j^{(P)} \times \begin{cases} \Omega_1 e^{i\kappa j a} - \Omega_2 & j \text{ odd}, \\ \Omega_2 e^{i\kappa j a} - \Omega_2 & j \text{ even}, \end{cases} + \sum_{j=1}^P k_{b,j}^{(P)} \times \begin{cases} \Omega_1 e^{-i\kappa j a} - \Omega_2 & j \text{ odd}, \\ \Omega_2 e^{-i\kappa j a} - \Omega_2 & j \text{ even}, \end{cases} \end{aligned} \quad (3.17)$$

As the angular frequency ω must have positive values, the quartic equation can be solved for $\bar{\omega} = \omega^2$. The solution for the two dispersion branches $\omega = \omega(\kappa)$ then reads

$$\begin{aligned} \bar{\omega} &= -\frac{1}{m}(-2D_1 + D_2 + D_3) \pm \\ &\pm \sqrt{\left(\frac{1}{m}(-2D_1 + D_2 + D_3)\right)^2 - 4\left(\frac{1}{m^2}(D_1^2 + D_2D_3 - D_1D_2 - D_1D_3 - D_4D_5)\right)} \end{aligned} \quad (3.18)$$

and substituting the $\bar{\omega} = \omega^2$ values in the equations yields the values of Ω_1 and Ω_2 .

Remembering that $k_{a,j}^{(P)} = k_j^{(P)} + \Delta k_j^{(P)}$ and $k_{b,j}^{(P)} = k_j^{(P)} - \Delta k_j^{(P)}$, and that $e^{ij\kappa a} + e^{-ij\kappa a} = 2\cos(j\kappa a)$, $e^{ij\kappa a} - e^{-ij\kappa a} = 2i\sin(j\kappa a)$ the coefficients of the dispersion relation can be reformulated, using the definition in equation 2.14, as

$$D1 = \sum_{j=1}^P 2 \frac{EV_{const}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} \quad (3.19)$$

$$D2 = \sum_{j=2}^{P_{even}} 2 \frac{EV_{const}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} (\cos(i\kappa a) + i\sin(j\kappa a)) \quad (3.20)$$

$$D3 = \sum_{j=2}^{P_{even}} 2 \frac{EV_{const}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} (\cos(i\kappa a) - i\sin(j\kappa a)) \quad (3.21)$$

$$D4 = \sum_{j=1}^{P_{odd}} 2 \frac{EV_{const}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} (\cos(i\kappa a) + i\sin(j\kappa a)) \quad (3.22)$$

$$D5 = \sum_{j=1}^{P_{odd}} 2 \frac{EV_{const}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} (\cos(i\kappa a) - i\sin(j\kappa a)) \quad (3.23)$$

in which the dependency on the stiffness distribution parameter α is explicit. The intermediate steps of the analytical derivation are available in A.2.

3.2.4 Periodic configuration of the defected mass-spring chain

Following the analytical analysis, a periodic mass-spring chain with N elements in the unit cell, with Bloch-Floquet boundary conditions is next considered. The chain considered as unperturbed multi-atomic, thus its dispersion relation entails multiple branches. The mathematical description of the general case is carried out in Appendix A.3, and an example lattice dispersion is shown in the Results section.

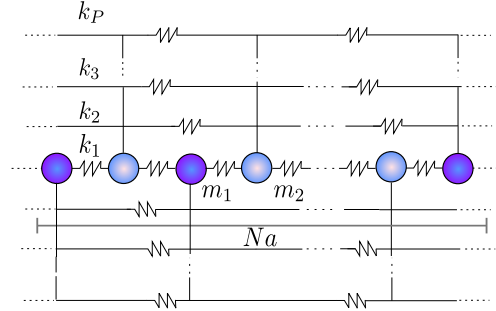


Figure 3.3: Unit cell configuration of the supercells with length Na .

3.3 Results and Discussion

In this section the results of the analysis both on infinite, periodic lattices and finite lattices are presented.

3.3.1 Dispersion curves for chains with odd atom masses

As for the monoatomic lattice, the dispersion curves will vary based on the stiffness distribution parameter α and on the nonlocality level P .

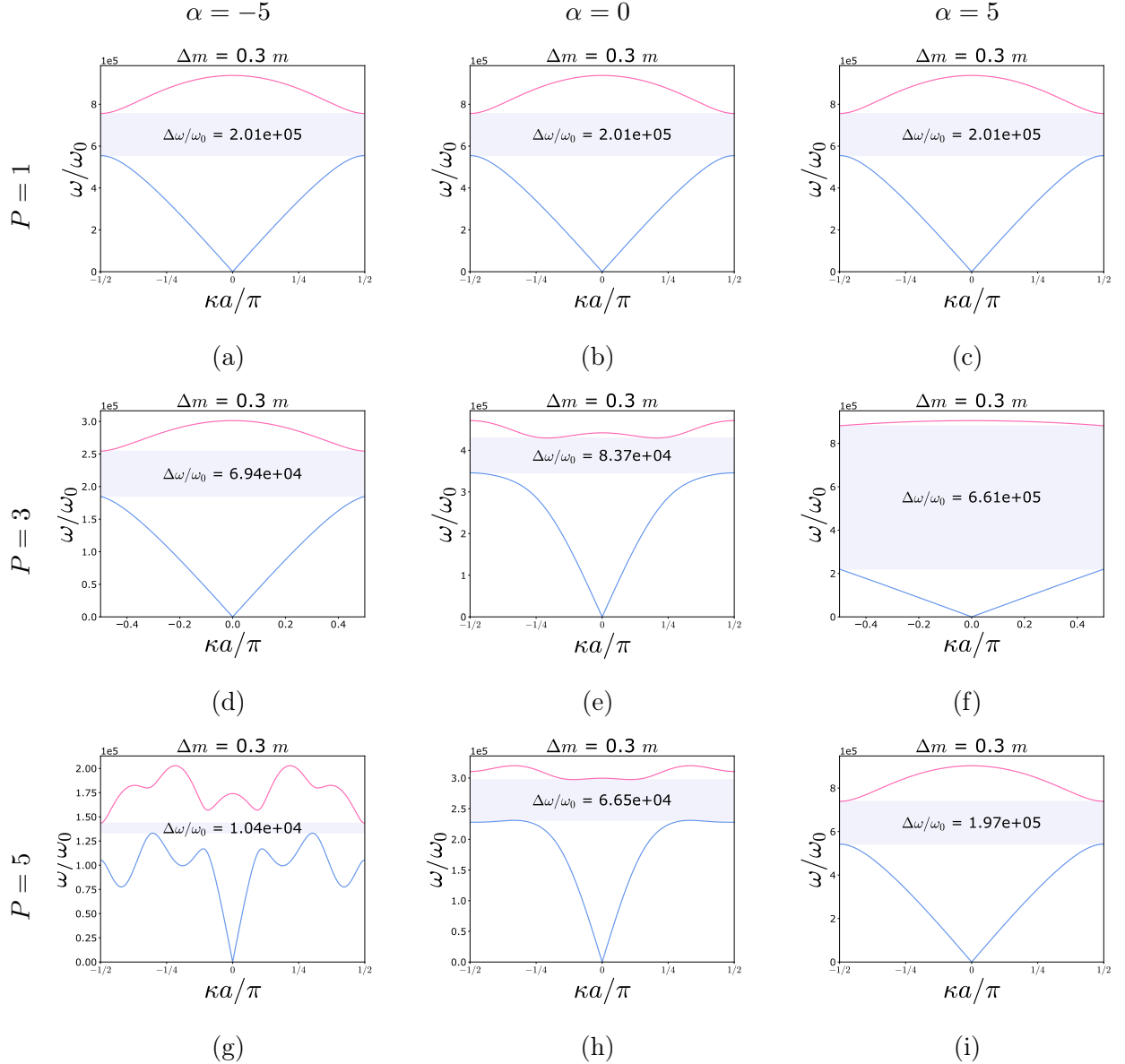


Figure 3.4: In this figure the dispersion relations are shown for 9 different α, P parameters, with a constant $\Delta m = 0.3$ value. It can be noticed that the band gap shifts in value but never closes when a difference between the value of the two masses in the unit cell m_1, m_2 is present. However, when local minima and maxima due to negative group velocities v_g are present in chains with $P > 1$ and $\alpha < 1$, the band gap reduces in some κ wavenumber ranges. The angular frequencies ω are expressed in $[\text{rad/s}]$.

Only, this time, as the unit cell length has doubled in size due to the mass shift, the first Brillouin zone is half its original size and the dispersion relation has two branches, one for the degree of freedom corresponding to $m_1 = m + \Delta m$ and one for $m_2 = m - \Delta m$, named the optical and the acoustical branches.

Figure 3.4 below shows dispersion curves for $P = 1, 3, 5$ and $\alpha = -5, 0, 5$ for the diatomic chain with $\Delta m = 0.3m$. The shifts in frequency range and slope in the curves display the effects of local and nonlocal connections on the mass-conserving diatomic chain. Figure 3.6 (a), (b) and (c) refer to the local case, therefore the value of the stiffness distribution parameter α has no impact on the resulting dispersion relation and bandgap, which is ruled by the Δm value. On the other hand, Figure 3.6 (f) and (i) present similar curves as the value $\alpha = 5$ hinders any nonlocal effects from taking place, advantaging the stiffness distribution onto the local links. Figure 3.6 (d), (e), (g) and (h) instead show dispersion curves that are impacted by the nonlocal couplings, where local minima and maxima surge both on the acoustical and optical branches. In particular, when $\alpha = -5$, the non-monotonicity of the curve causes the bandgap to shrink, which could be employed in targeted frequency attenuation.

3.3.2 Transition between diatomic and monoatomic lattice

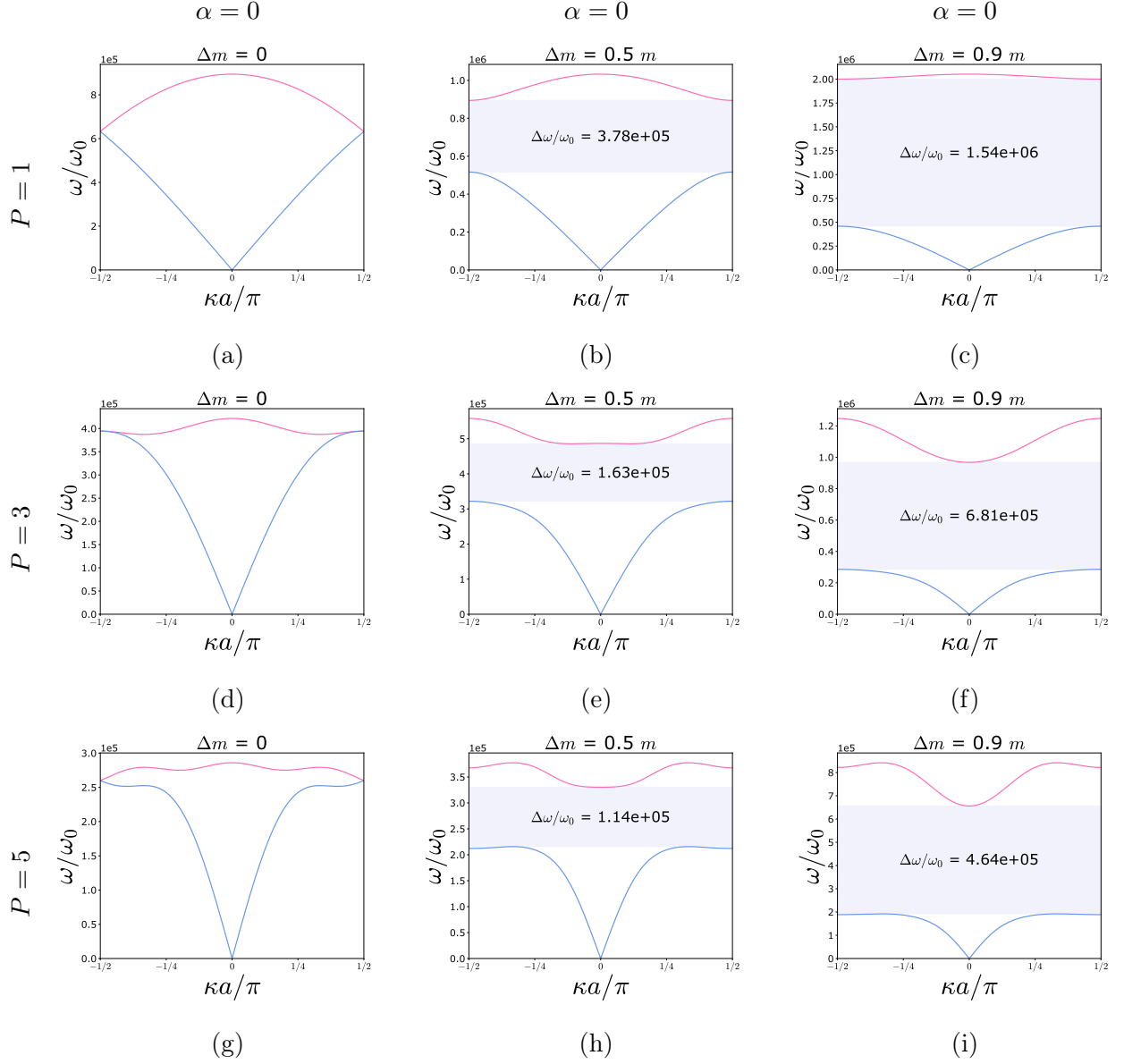


Figure 3.5: In this figure the dispersion relations are shown for 9 chains with different values of the parameter P and $\alpha = 0$, with several mass-distribution configurations inside of the unit cell, i.e. different Δm values. As the Δm value increases, so does the band-gap size, while when Δm goes to zero the band-gap closes. The angular frequencies ω are expressed in [rad/s].

When $\Delta m = 0$, the diatomic configuration is lost as the band gap closes and the two branches correspond to the folded acoustical branch of the monoatomic dispersion curve, the bandgap closes and the monoatomic solution can be retrieved as shown in the introduction to this thesis. On the other hand, when the difference in mass between the atoms in the diatomic unit cell increases, the band-gap increases accordingly.

Figure 3.5 below illustrates the transition between a diatomic and a monoatomic chain, explored in terms of percentage of mass shifting from an element to another in beads.

3.3.3 Dispersion curves for chains with odd springs' masses

In Figure 3.6 the dispersion relations of the diatomic chain with fixed stiffness odd distribution $\Delta k_j^{(P)}$ is illustrated for values of $\alpha \in [-5, 0, 5]$. The band-gap shape and width depends on the roton-like configuration of both the acoustical and optical branches, and predicting the result is not trivial. In particular, Figure 3.6 (g) highlights a case where, albeit diatomic, the chain does not feature a continuous band-gap because of the local minima and maxima being uneven.

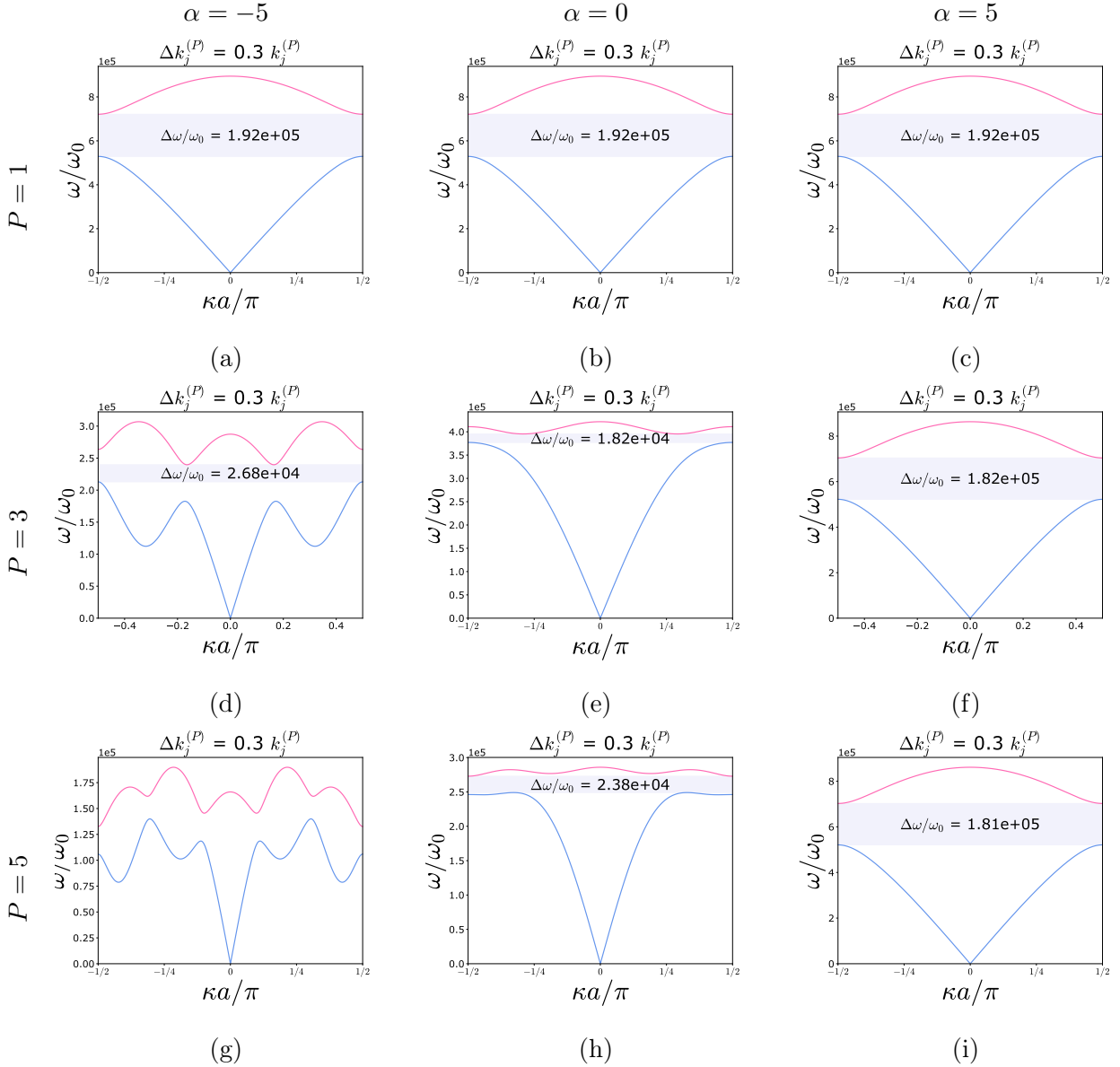


Figure 3.6: In the 9 graphs above, the dispersion relations for a diatomic lattice with mass shifts in the m_s springs' masses are shown. Every graph refers to a $\Delta k_j^{(P)} = 0.3k_j^{(P)}$ distribution. The band-gap width and length varies with the P, α parameters combinations, but as long as the stiffnesses of the springs' to the right and to the left of each mass in the unit cells are different, the optical and acoustical branches remain separate. The angular frequencies ω are expressed in [rad/s].

3.3.4 Mass shifts and band gap width

In Figure 3.7, the transition between a diatomic and a monoatomic one-dimensional lattice is illustrated for $\alpha = 0$ and stiffness distribution disparity varying in $\Delta k_j^{(P)} \in [0, 0.5, 0.9]$. When the springs on the right and on the left of each mass are equal for every level of nonlocality, the chain turns monoatomic, therefore in Figure 3.7 (a), (d) and (g) reflected branches of the dispersion relation are shown due to the doubling of the size of the first Brillouin zone.

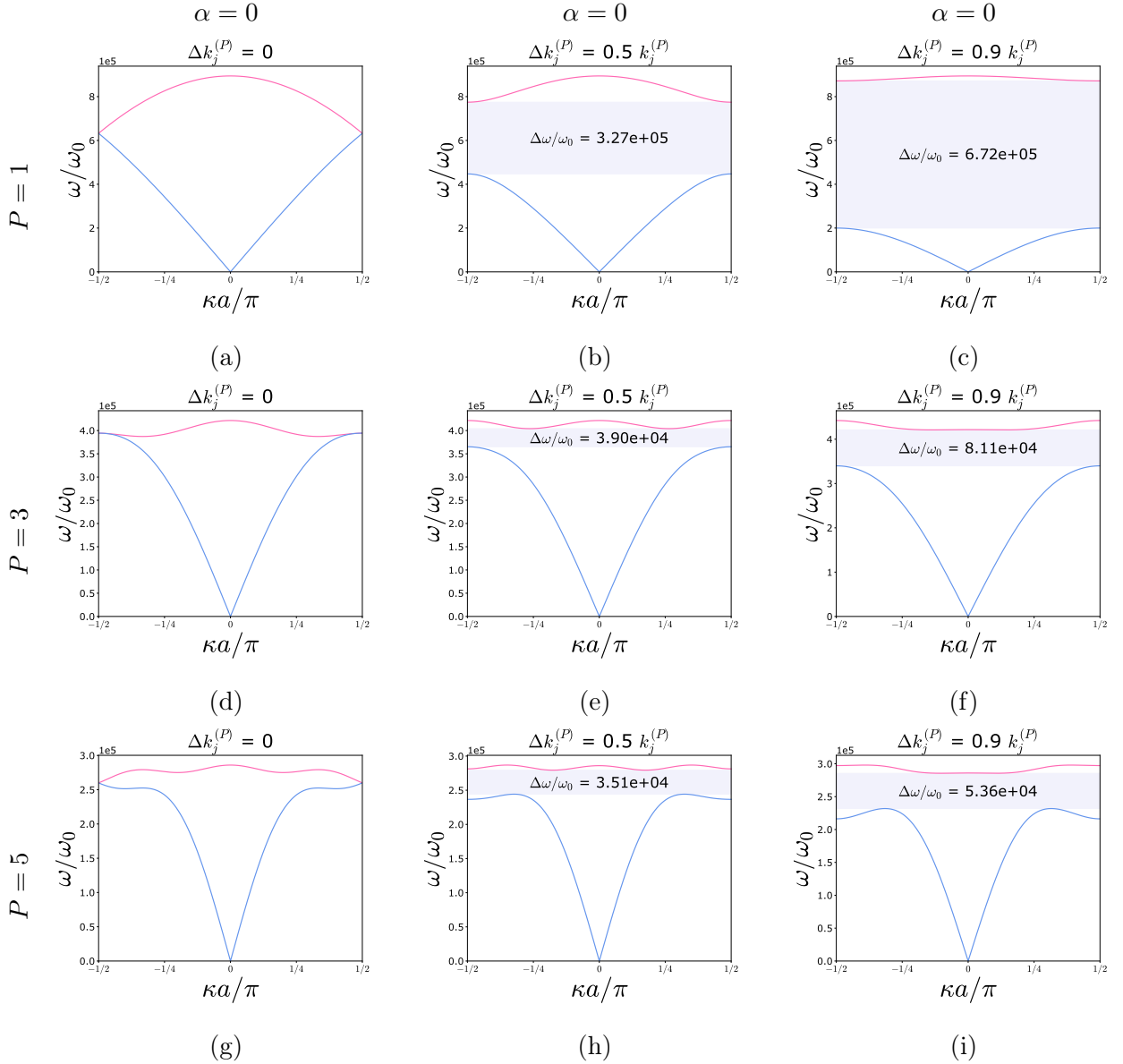


Figure 3.7: In this figure the dispersion relations are shown for nine chains with different values of the parameter P and $\alpha = 0$, with varying springs' mass distribution leading to uneven springs' stiffnesses to the right and to the left of each mass in the unit cell. When $P > 1$ and $\alpha < 1$, the dispersion curves show a roton-like behaviour, while the bandgap width and length depends on the $\Delta k_j^{(P)}$ values. The angular frequencies ω are expressed in $[\text{rad/s}]$.

3.3.5 Conditions on the mass-shifts among the atoms

The mathematical formulation of non-locally connected one-dimensional chains has been so far based on a core idea that revolves around maintaining a physically sound mass ratio between the particles and the springs in the unit cell. This is obtained by keeping a constant amount of material when introducing BNN couplings. As the springs' material is considered to be homogeneous, this is achieved by applying a volume conservation law for elastic springs. This means that when additional spring connections are added to create a nonlocal chain, the total volume (and therefore mass, assuming constant density) of the spring material remains the same as in the local model.

The model assumes that the mass of the springs is negligible and does not contribute to the dynamics of the chain. When $m_2 \approx m_s$, and thus $\mu \approx 1$, the model's assumption of negligible spring mass would no longer hold, and the inertia of the links would need to be included in the calculations.

Therefore a constraint is imposed on the possible defected configurations, that at least one order of magnitude separates the values of the beads' and the springs' masses.

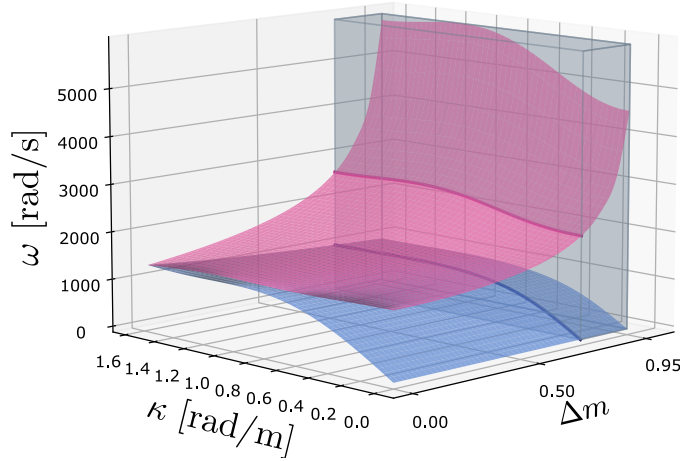


Figure 3.8: In the figure above, every κ, ω plane represents a dispersion relation for a different Δm value. As the difference between $m_1 = m + \Delta m$ and $m_2 = m - \Delta m$ increases, the band-gap between the acoustical branch and the optical branch, respectively the green and pink surfaces, enlarges. On the other hand, when $\Delta m = 0$ the band gap closes. The grey polygon indicates the Δm values where $m_2 \approx m_s$ in every unit cell, therefore implying that the mechanical consistency condition is no further valid. This area is thus considered to provide invalid solutions.

3.3.6 Example of a diatomic chain with multiatomic unit cell

As anticipated, a unit cell with two masses in it generates a dispersion relation with two curves, the acoustic (lower) and the optical (upper) branch, and a band gap in between, whose frequency and width depend on the mechanical characteristics of the lattice. In this case, a unit cell with N masses is considered, although in the non-defected case a unit cell with two masses would be sufficient to depict its dynamic behaviour. The first Brillouin zone depicts the smallest symmetrical area in the reciprocal space (frequency domain), which corresponds to $d = \pi/a$, a being the length of the unit cell considered in the direct lattice. As in this case the unit cell considered is larger than the smallest symmetrical unit, the Brillouin zone will be smaller than it should be, causing the graph to show N folded branches.

3.3.7 Periodic lattice, defects and localised modes

In the following Figure 3.9, the resulting dispersion relation is shown for a local system and two nonlocal ones, with respectively $P = 1$, $P = 3$ and $P = 5$, for three different values of the stiffness distribution parameter α . The chains are considered to include $N = 10$ atoms in the unit cell for illustrative reasons, albeit only two different, alternated mass values are present, m_1, m_2 . Figure 3.9 therefore shows *folded* branches both for the acoustical and optical part, as the first Brillouin zone is considered to be smaller than the minimum periodically repeated unit, and it is inversely proportional to the lattice constant a .

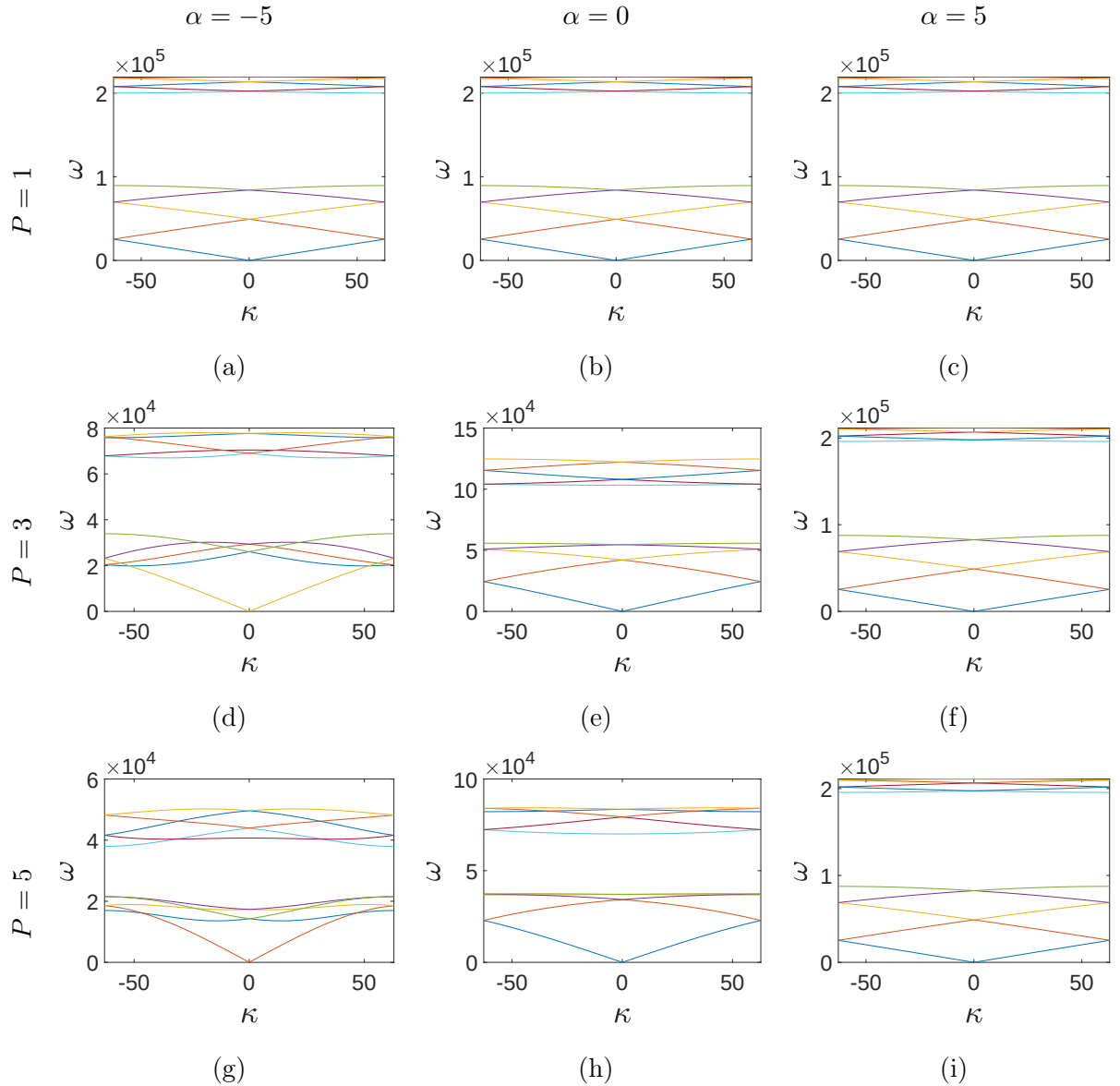


Figure 3.9: In this figure the dispersion relations are shown for 9 chains with different values of the parameter P and α , and $N = 10$ masses in the unit cells. As the masses have values m_1 and m_2 , the smallest unit cell would only include two, therefore only two branches in the dispersion relation, optical and acoustical. Thus, there is a reflection of the first Brillouin zone which is considered smaller than it actually is, i.e. $BZ \in [-\pi/10a, +\pi/10a]$ instead of $BZ \in [-\pi/2a, +\pi/2a]$

3.3.8 Finite chain simulation: numerical dispersion curves through the 2D Fast Fourier Transform

In order to observe the effects of the defects on possible prototypes to be manufactured, a numerical analysis has been carried out. In particular, there is an issue that presents itself with periodic media with nonlocal connections. As the chain is envisaged as infinite periodic in the analytical analysis, the nonlocal connections are equal in each and every unit cell, however, when the infinite periodicity hypothesis is removed, there will be a different level of nonlocal connections at the boundaries of the system compared to the bulk. It is thus necessary to consider an adequate number of nonlocal connections to neglect the boundary effect.

To maintain a reasonable computational cost while preserving the key features of the model and avoiding boundary effects, a chain of 500 masses, aligned along one direction. The ends are fixed, in order to ensure full reflection, and only the longitudinal vibration, i.e. axial displacement degree of freedom, is admitted. The chain is excited by a harmonic force applied at its center, employing a chirp modulation that spans the resonance frequencies of the system. The numerical simulations are implemented in *Python* and consist of two steps. The first one is an explicit dynamic simulation under external forcing, and the system is solved iterating the time-steps in Newmark's method [14]. The initial conditions were set to zero, meaning no initial acceleration ($\ddot{\mathbf{U}} = 0$), velocity ($\dot{\mathbf{U}} = 0$), or displacement ($\mathbf{U} = 0$) was imposed on any mass. The mass matrix ($\mathbf{M}$) and stiffness matrix ($\mathbf{K}$) for the finite system were constructed, accounting for the fixed ends. A time-varying force, with a chirp modulation in frequency, was applied to the central mass to reconstruct the dispersion curves by capturing the system's response across most of its eigenfrequencies. Afterwards, the resulting displacements in the time domain are translated in the frequency domain through two-dimensional Fast Fourier Transforms (2DFFT), which yield the numerical dispersion relation of the lattices in the frequency domain. Finally, the 2DFFT were sampled in a binary way, discarding the response amplitude information in order to focus on the dispersion shape.

The numerical simulations are carried out for two different configurations. The first one is diatomic, with a mass shift imperfection equal to $\Delta m = 0.3$. As mentioned earlier, this will yield a numerical dispersion relations with two branches, and the first Brillouin zone is not set a priori and is retrieved from the frequency domain results. The second one features a localised defective item in the middle in addition to the Δm induced one.

3.3.9 Diatomic lattice

In the first round of simulations the system is considered not to have any imperfections. Figure 3.11 shows the dispersion relations yielded by the numerical simulations and 2D FFTs on this chain. The results are shown for different values of α and P . The dispersion curves are retrieved for the biatomic chains on both acoustic and optical branches for nonlocal chains ($P > 1$) with several α values.

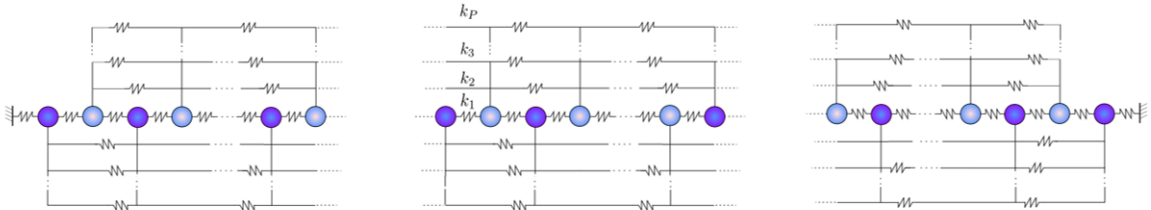


Figure 3.10: *Finite diatomic configuration, with fixed ends.*

Figure 3.11 (a) and (d) represent the cases case where non-local interactions are significant, leading to roton-like dispersion curves. These curves are characterised by accentuated local minima and max-

ima, as per analytical prediction. Figure 3.11 (b) and (e) show dispersion curves with an intermediate value $\alpha = -0.5$, showing a transition between local and non-local behaviours. Figure 3.11 (b) and (e) correspond to a predominantly local interaction regime with $\alpha = 5$, where the dispersion curves are more similar to those of a simple diatomic chain.

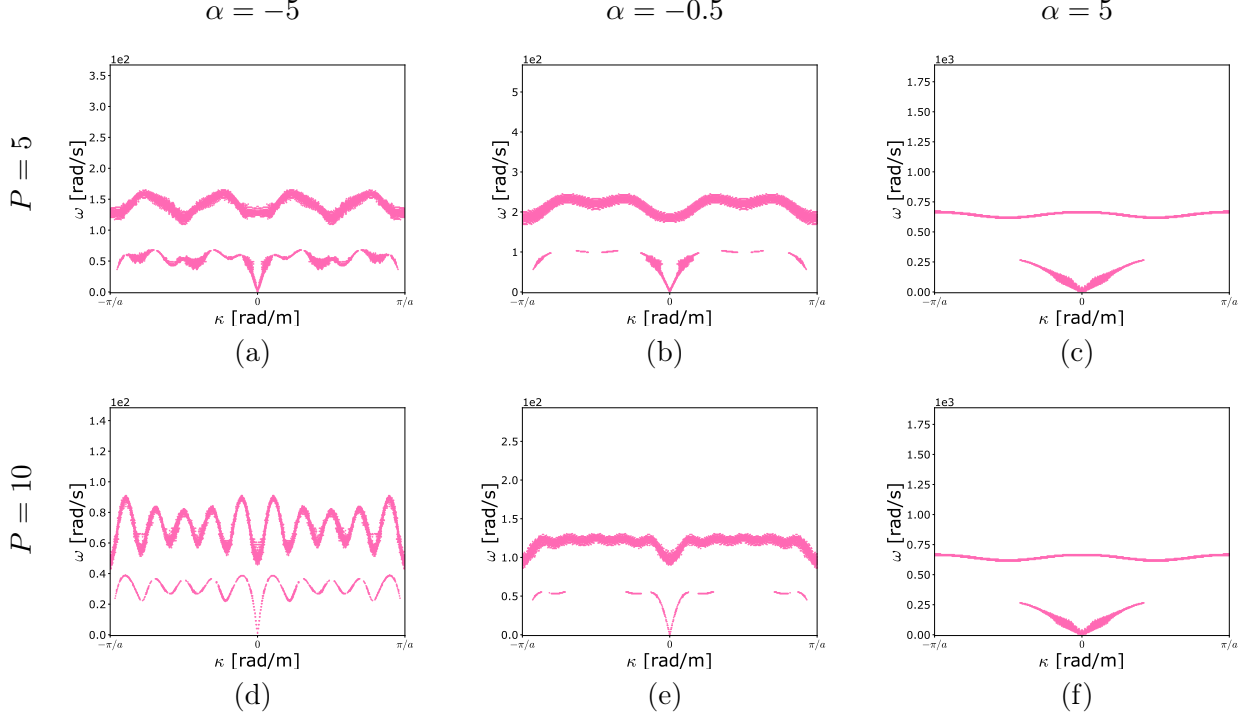


Figure 3.11: In this figure, the numerical dispersion relations of the $N = 500$ masses chains with fixed-fixed boundary conditions are shown. The 2D dispersion curves are extracted from the frequency domain by reducing the information to a binary distinction between frequencies excited and not in the response, thus no information on the vibration amplitude is displayed above.

3.3.10 Some numerical insights: diatomic finite chains with a localised imperfection

The trial configuration shown here entails a diatomic chain of alternated masses with a defective unit in the middle, and has only been numerically studied.

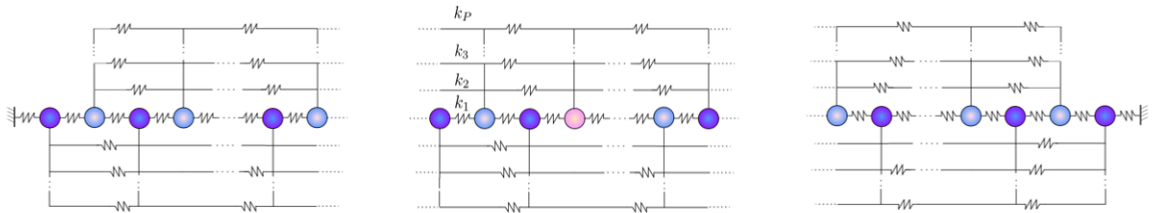


Figure 3.12: Finite diatomic configuration with a localised imperfection, with fixed ends.

In this case, a clear localised mode can be retrieved at any nonlocality level P and α value, as shown in Figure 3.13. In order to generate an illustrative imperfect lattice, a defected mass is inserted in the 250^{th} position of a unit cell with $N = 500$. This causes an additional branch of the dispersion relation to appear, representing the third mass added to the previous two.

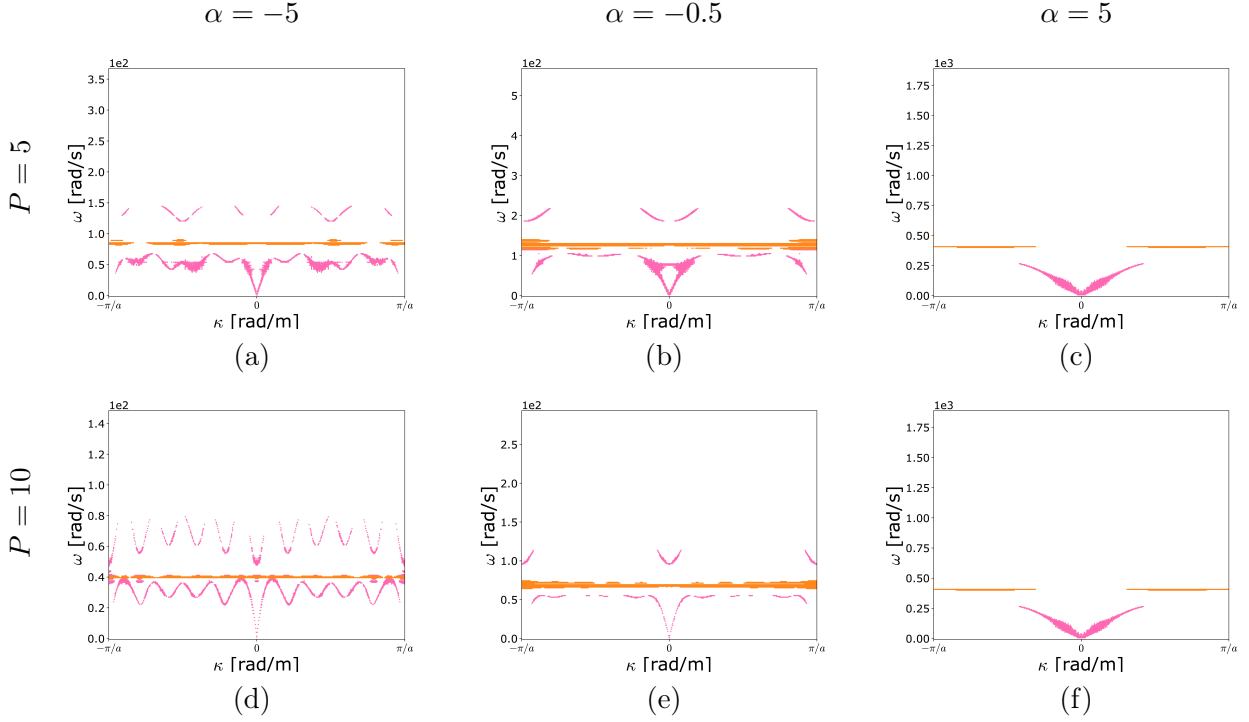


Figure 3.13: In this figure, the numerical dispersion relations of the $N = 500$ masses chains with fixed-fixed boundary conditions are shown. The 2D dispersion curves are extracted from the frequency domain by reducing the information to a binary distinction between frequencies excited and not in the response, thus no information on the vibration amplitude is displayed above. The chain is constrained at both ends, the masses being alternated with m_1, m_2 values by adding or subtracting $\Delta m = 0.3m$, and $m = 1\text{kg}$, and the constants $E = 23\text{GPa}$, $V = 0.1\text{m}^3$, $a = l_0 = 0.005m$. Input parameters entailed input force $F = F_0 \cos(\omega(t))$, where $F_0 = 1\text{N}$ and forcing frequency ω varying at each time step through a chirp modulation, in the range of the natural frequencies of the chain.

3.3.10.1 Imperfections and energy shifts

The aim of this part of the work is to quantify the effects of defective elements in periodic lattices in terms of energy, and compare the results to examine the impact of the number and strength of nonlocal connections onto the energy distribution. To do so, the energy contents of the chains under harmonic forcing are retrieved from the problem data and the explicit dynamics simulations, i.e., the displacement values along the lattice. The total energy is considered to be split into two components: the elastic energy, E_{el} , and the kinetic energy, E_k . It is thus defined as follows

$$E_{tot} = E_{el} + E_k, \quad (3.24)$$

where

$$E_{el} = \frac{1}{2} \sum_{j=0}^{(P)} k_j^{(P)} (x_n - x_{n+j} - x_{n-j})^2 \quad (3.25)$$

and

$$E_k = \frac{1}{2} m \dot{x}_n^2. \quad (3.26)$$

In this context, it is hypothesised that the elastic energy E_{el} belongs to the n_{th} mass exclusively, in order to allow for a rough comparison between configurations.

Figure 3.14 illustrate the energy distribution difference on elements when a mass distribution shift happens or not. This is calculated both for odd and even items, and energies are retrieved from the explicit dynamic simulations. Figure 3.14 (a) and (c) show the energy difference for nonlocal chains with respectively $P = 5, 10$ and $\alpha = -5$ in both cases. A greater quantity of energy being absorbed and released is to be detected compared to Figure 3.14 (b) and (d), where regardless of the level of nonlocality local links are predominant, due to the $\alpha = 5$ value.

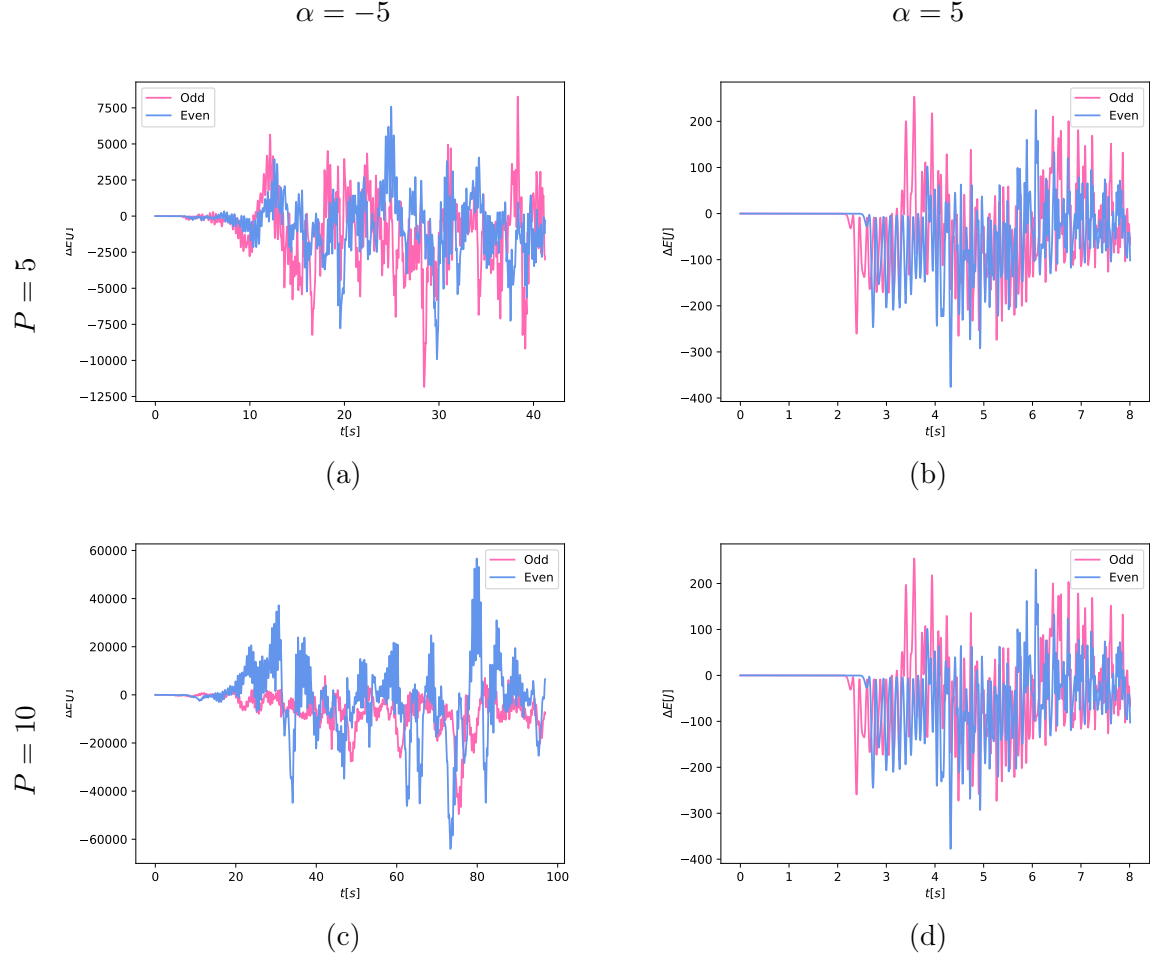


Figure 3.14: In this figure, the difference in total energy E_{tot} between the defected and intact configuration of two monoatomic-diatomic lattices is shown. The pink curves in both graphs refer to the energy content of the odd element in the unit cell, that is, the difference in energy content between the non defected and defected mass on the same position. The blue curve instead represents the difference in energy between the defected and intact lattice, calculated onto the even mass in the unit cell. It can be observed how both in (a), (b), (c) and (d) there is a significant absorption and release of energy in the defected masses when the chain presents an imperfections.

3.3.10.2 Energy localisation analysis

Subsequently, the localisation phenomena in infinite and finite mass-spring chains have been studied in terms of energy. The simulation and evaluation procedure is the same of the one carried out above in ??, however in this case the mass to which the input forcing is applied to is characterised by a localised imperfection, i.e. it is different in value from the two masses of the diatomic configuration.

The energy evaluation shows that the absolute value shift in energy are concentrated into a narrower period of time, which, as per the excitation conditions, corresponds to a specific frequency range. This can be interpreted as energy shifts being localised to a set of degrees of freedom, i.e. masses, more or less close to the defected item based on the nonlocality level P . This can be clearly observed in the graphs below, where the local case results in a jump in energy value concentrated in time, while the nonlocal configuration calls for the participation of more masses into the motion at the resonance frequency of the defected item, leading to a more distributed energy shift. In Figure 3.15, two plots are presented. In both of these graphs the difference between a defected and an intact chain is presented in terms of energy calculated on single mass, in orange for the one that becomes defected, and in blue for one that keeps its value in the imperfect configuration. Figure 3.15 (a) refers to a strongly local chain, as the positive value of the stiffness distribution parameter α makes the nonlocality level P negligible, while Figure 3.15 (b) refers to a chain with a nonlocal, roton-like behaviour due to the negative α value. In both cases it can be observed how the total energy E_{tot} levels remain constant, i.e. do not jump, passing from the perfect to imperfect configuration when measured on a mass that is not defected (blue curve). On the other hand, when the energy levels are observed for a mass which changes its value from a configuration to another, a significant value oscillation is observed.

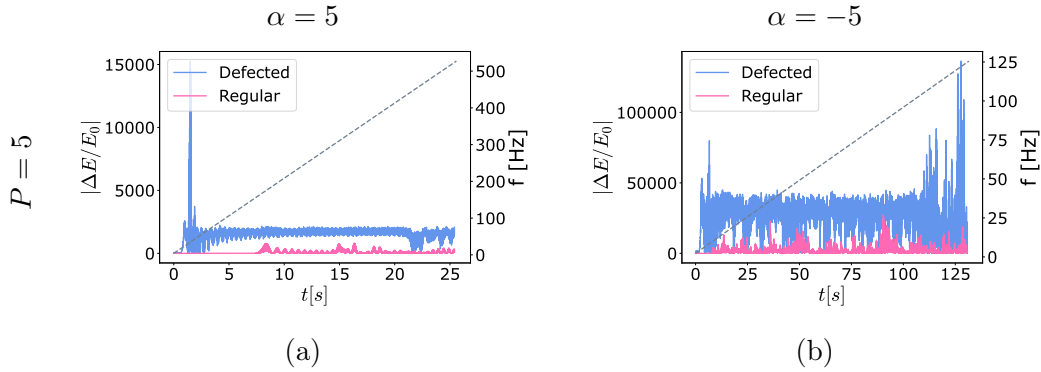


Figure 3.15: In this figure, the difference in total energy E_{tot} between the defected and intact configuration of two diatomic lattices is shown. The orange curves in both graphs refer to the energy content of the defected unit, that is, the difference in energy content between the non-defected and defected mass on the same position. The blue curve instead represents the difference in energy between the defected and intact lattice, calculated onto a non-defective mass, that is, one mass that keeps its value constant in both configurations. It can be observed how both in (a) and (b) there is a significant absorption and release of energy in the defected mass when the chain presents an imperfection, while the energy levels remain unchanged on other masses on the lattice.

This study explores the impact of mass-shift induced defects within mass-conserving, nonlocal one-dimensional chains, in order to account for manufacturing inaccuracies that are unavoidable for metamaterials, theoretically periodic structures. The *mechanical consistency* condition ensures a physically consistent model, retraining the overall springs's masses as it would not be negligible otherwise in a nonlocal regime. By considering a constant overall mass of elastic links, the model can also be used to compare different metamaterial designs. In this case the defect is originally defined as a disparity in mass distribution, which hinders the lattice symmetry. However, the analysis is here limited to subsequent elements, leading to the creation of a perfectly periodic diatomic lattice. With the aim of exploring a broader distribution of defects, a future perspective of this work could lead to the application of the same concept to a larger area, exploring different mass distribution configurations. In particular, when the springs' masses are concerned, it would be interesting to evaluate the effects of a defective configuration that locally flips the value of the stiffness distribution parameter α over, creating a localised local or nonlocal configuration. Localised defects can be in fact a hindering to

wave propagation, but also an asset for energy harvesting, as they can lead to energy capturing in the defected area. Works as the one by Zhao et al. [93] explored the effects of localised modes on a finite lattice, however the parameter choice to reach the desired energy distribution is discussed only for selected configurations (involving geometry and rotation of the defect) and in the local case. A framework which involves nonlocal couplings with specific control parameters is still to be developed. The first insights of a possible follow-up of this work are discussed in section 3.10, where localised modes are attained numerically in locally defected mass-conserving chain. An analytical treatment of the problem, for instance considering the topological implications on an infinite chain, as discussed by Miniaci and Pal [103] and Dal Poggetto et al. [34] would perhaps be beneficial to a further understanding of the problem, providing further quantitative parameters and results to better understand the dynamical implications and the design possibilities of rendering periodic lattices locally defected or quasiperiodic. Moreover, this model is limited to one-dimension, however the same framework could be employed in the design of waveguides and directional filters by employing two- or three-dimensional structures. Finally, the effects of localised nonlinearity could be investigated when the nonlinear behaviour is confined to a specific area.

3.4 Conclusions

The previously proposed mass conservation criterion [120] is here extended to diatomic one-dimensional lattices. The diatomic configuration of the unit cell emerges from a *defected* state, given by a localised shift of symmetry in the mass distribution, with it being inhomogeneous between two consecutive masses or springs. This causes the dispersion relation of the chain to be formed by two branches, with a band gap which closes when the mass distribution difference in masses or springs disappears. By rewriting the dispersion curve within the doubled first Brillouin zone, the monoatomic nonlocal dispersion relation can be retrieved. In the numerical simulations, a further inaccuracy in the mass distribution is considered. An additional band appears in the dispersion curve, namely a localised mode, as seen in other works on the subject matter in literature, cited in the Introduction to this chapter. Energy consideration are made on both specimen, in order to quantify the energy harvesting potential of possible diatomic unit cell metamaterial devices.

All in all, a roton-like multiple-branch dispersion relation is yielded for any level of nonlocality. The model obeys the *mechanical consistency* condition previously proposed by the authors, thus ensuring the coherence of the mass spring model with its physical prototype. Further analyses on defected lattices could be helpfully employed in waveguiding and energy harvesting devices.

Chapter 4

Towards nonlinearity: perturbing linear elasticity in nonlocal systems

Abstract

Dynamics of periodic structures and quasi-crystalline lattices is attracting a growing interest in physics and engineering at different scale levels and for a wide range of applications. Very recently, nonlocal metamaterials have been repropounded by adding, in the lattices, multiple beyond nearest neighbour couplings among elements to obtain dispersion relations allowing for roton-like behaviours and phase and group velocities with opposite signs. Moreover, metamaterials with nonlinear pairings have been studied in the attempt to increase the tailorable features, e.g., through amplitude dependent frequency responses and therefore enhance the design spectrum for wave-manipulation devices. However, mathematical models and real prototypes in literature seem neither to provide criteria to compare local and nonlocal lattices nor to discuss any related rules governing the transition between the two configurations. In this framework, the present study extends a previously proposed conservation law for the elastic connections in mass-spring systems by the present authors, which are the most employed building blocks for a vast number of metamaterials. The relationship between nonlocality and nonlinearity in a one-dimensional monoatomic chain is here investigated. The conservation law is enforced for nonlinear couplings, so the level of nonlocality P and the stiffness distribution parameter α are used to govern the design of the nonlinear nonlocal chain. Effects of weak cubic nonlinearities are observed through perturbation techniques. The results attained are employed to yield perturbed and nonlinear amplitude-dependent dispersion relations for nonlocal, mass-preserving monoatomic chains. Finally, a numerical validation is carried out.

4.1 Introduction

Nonlinear systems exhibit complex behaviors that do not adhere to the same set of rules linear systems do, and the prediction of the outcome of their behaviour is decidedly more challenging. Even though linear approximations are an invaluable tool for understanding the root of physical phenomena, real world applications, devices and projects often require nonlinear analysis in order to be reliable. In fact, especially in dynamics, when nonlinearity arises, unpredictable outcomes can take place when it is not accounted for. Most importantly, nonlinearity opens doors to novel phenomena and allows for engineering materials and structures with tailored responses. It can entail chaos and sensitivity to initial conditions, bifurcations in dynamical behaviour and amplitude dependent responses, energy trapping and localization phenomena, properties that can pave the way to novel developments.

In mechanical systems, nonlinearity can arise from several sources, such as constitutive laws (stress-strain relationships), geometric aspects, contact or impact conditions.

In a very recent review paper by Patil and Matlack [121], nonlinearity in mechanics is extensively discussed. The authors focus above all on the wave responses that are outside of the linear dynamics spectrum, and on the sources of nonlinearity needed to achieve them. The cited sources of nonlinearity are the following:

1. Nonlinear force-displacement relationships of spring stiffness;
2. Material nonlinearity, i.e., nonlinear stress-strain relationship;
3. Geometric nonlinearity (multistability, configuration);
4. Contact nonlinearity, e.g. Hertzian power laws;
5. Nonlinearity arising from a combination of the above mentioned factors.

The points 2. and 3. are especially important as they can arise both from manufacturing imperfections or the material used in certain applications, as for instance flexible and bio-inspired materials can easily branch out to nonlinear deformation ranges. Point 2 also comprehends *constitutive nonlinearities*, including nonlinear elastic potentials, which allow materials to undergo large deformations with a nonlinear stress-strain ratio. Among others, some common nonlinear elastic potentials are the hyperelastic models as the Neo-Hookean and Mooney-Rivlin. A commonly used potential for hyperelastic materials is the Murnaghan potential ([122], [123]).

In nonlinear dynamics, however, these constitutive laws are not always taken into consideration. The typical investigation of the dynamic response of nonlinear media and devices involves considering polynomial stiffness functions and analysing the impact of quadratic and cubic nonlinearities, and wave-wave interaction phenomena ([124], [125], [30], [126]).

4.1.1 Nonlinearity in dynamics

In the dynamics realm, nonlinearity can give rise to interesting phenomena which evade the traditional linear systems rules and methods. For instance, eigenvalue and matrix based methods, such as Fast Fourier transforms, plane wave expansion or transfer matrix method are no longer applicable [127].

Based on the degree of nonlinearity, i.e. whether it is weak or strong compared to the other quantities at play, semi-analytical approximations as perturbation methods [128] or numerical methods as direct integration can be employed both in the time and frequency domain.

Apart from the instruments, the traditional information on dynamics response from the physics of linear systems is no longer valid. For instance, vibration modes can intertwine, in contrast to the linear case in which they are always decoupled. Another characteristic of linear wave propagation is reciprocity, that is the invariability of response if inverting the source and the receiver. This property can be lost in nonlinear media, which can be nonreciprocal in wave transmission. Furthermore, phenomena induced by nonlinearity include solitary waves propagation (solitons), in different forms, such as pulses and breathers [129].

Moreover, nonlinear responses to harmonic and anharmonic forcings can entail mode bifurcations and multistability, and erratic, aperiodic responses when the system's behaviour becomes chaotic, i.e. highly dependent on the initial conditions in an unpredictable way. A thorough explanation of the physical concepts underlying chaotic behaviour is to be found in the book by Strogatz on the subject matter [130]. While even chaotic behaviour from nonlinearity offers immense potential, it presents the challenges that come with strong nonlinearity. Modelling, predicting behaviour, and designing nonlinear devices which exploit chaotic responses requires advanced techniques. In this seminal paper Vakakis [131] demonstrates the existence of chaos and dependence on initial conditions of nonlinear

systems, as there exists an array of degenerate resonance frequencies. Hu et al. [132] applied the Harmonic Balance Method to retrieve the Duffing oscillator solution. This method is often employed to approximate nonlinear behaviour through sinusoidal functions and a book by Krack [10] provides an extensive guide to the Harmonic Balance Method and its applications to classical mechanical systems.

One of the fields in which chaos opens new perspectives is energy harvesting. Telles Ribeiro et al. [133] developed an enhanced feedback control method to recover voltage signals from chaotic energy harvesters at low energy expenditure. De la Roca et al. [134] instead focus on exploiting the chaotic behaviour of the system for energy harvesting purposes. In fact, the power generation of piezoelectric harvesters can be enhanced by nonlinearities, both for signal quality and amplitude, when resonance frequencies are not hit. However, the response of the harvesting devices should still be stable and controllable, therefore the authors developed an active system to keep the dynamic response of prescribed orbits and periods.

In the recent paper by Li et al. [135] the vibration properties of graphene shells are investigated when nonlinearity and chaos come into play.

4.1.2 Nonlinearity in metamaterials

In the metamaterials community, nonlinearity has generated strong interest for its potential implications and applications in metamaterial designs. In mechanical metamaterials the dynamic response and wave propagation behaviour plays a pivotal role, and the addition of nonlinear components, albeit reducing the predictability of the response, enhances the spectrum of the possible outcomes. It is believed that being able to exploit these features could offer unprecedented functionalities and tuning possibilities. Generally speaking, metamaterial devices are often employed in vibration attenuation, wave manipulation and noise control. Nonlinearity in metamaterials can, for instance, be employed for energy harvesting or absorption, or on the other hand, for shock dissipation. For instance, Bukhari et al. [136] investigated the role of nonlinear local resonators on linear chains, and their impact on bandgaps formation, showing that they can induce shifts at low frequencies. Their linear counterparts generally respond better when resonance frequencies are entailed, while in other cases the nonlinearity can be a helpful tool to enhance the mechanical response. Furthermore, nonlinearities allow for the modulation of dispersion relations, as nonlinearities can provoke mixed frequencies and a shift in the frequency spectrum, tied to the amplitude dependency of nonlinear wave propagation.

Nonlinearity even leads to the surge of solitons, that are localised waves that maintain their waveform in spite of propagation and time evolution. They may serve the purpose of information and energy transmission. This can be helpfully employed, among others, in shock absorption and vibration damping.

Nonlinearities in metamaterials, as in regular systems, can be studied according to the degree of nonlinearity they are characterised by, be it weak or strong, thus allowing for semi-analytical methods or requiring numerical procedures.

4.1.3 Weak nonlinearity

When the nonlinear components of the system are negligible in magnitude and effects with respect to the linear components of the system, the dynamic response can be approximated to that of a linear system with a perturbation range. This is the case of weak nonlinearity, for which it is often possible to find analytical harmonic solutions.

In weakly nonlinear systems, a perturbation approach yields reliable results in the case of small amplitude forcing, if carefully employed. A thorough dissertation on perturbation methods cited in the following text is contained in the classical book by Nayfeh and Mook [128]. Both the Lindstedt Poicaré asymptotic expansion method and the Multiple Scales method can be employed in order to achieve

perturbation of dispersion curves due to different kinds of nonlinearity and wave interactions scenarios. Narisetti et al. [137] applied perturbation methods to periodic media, namely to a monoatomic chain with cubic nonlinearity. Other works on this topic followed, as cubic nonlinearities are the most commonly employed. Quadratic nonlinearities [138] can be treated with perturbation methods as well, however they are less commonly inserted into dynamic models as it is necessary to include high perturbation orders to see their effects on the frequencies and amplitudes of the response.

Weak nonlinearities can also result in amplitude induced bandgaps [139]. Furthermore, some wave mixing phenomena can take place when the nonlinearity causes self-interaction, as investigated by [126] through the Multiple Scales method. The authors studied the wave-wave interactions in a nonlinear one-dimensional monoatomic chain, where the nonlinearity stems from the cubic restoring force of the springs. Their work highlights the importance of understanding the frequency and amplitude dependent interactions in nonlinear metamaterials as they differ from their linear counterparts where only constructive and destructive interference can arise. In this case, super- and sub-harmonics emerge. This is of utmost importance when designing wave manipulation devices, where nonlinearities have a prominent impact on the propagation qualities. The authors employed a perturbation approach to analyse the dynamic response of the system, and illustrated the Method of Multiple Scales as a reliable tool to find dispersion curves as opposed to the Linstedt-Poincaré method, which is found only to be valid in the long wavelength limit and for time-invariant wave amplitudes. Wave interaction arising from local resonances was instead studied by Fronk and Leamy in 2019 [140]. The authors proved that in periodic chains and metamaterial lattices an internal resonance mechanism can take place when nonlinear plane waves interact with each other. Their analysis is carried out semi-analytically through the Multiple Scales perturbation method.

Vakakis and King [141] studied the dynamics of monocoupled periodic systems as early as in 1995, showing that as for their linear parallels, they possess attenuation and propagation zones, which correspond respectively to synchronous and asynchronous motion of particles. The investigation is carried out analytically through perturbation methods, i.e. the multiple scales methodology, expanded to periodic media.

Regarding pressure waves, Sugimoto and Horioka [142] examined the dispersion properties of sound waves in a tunnel with an array of Helmholtz resonators. They individuated stopping bands of acoustic Bloch waves that do not depend on dissipation but on resonance with the Helmholtz resonators. In a subsequent work, Swintek et al. [143] applied perturbation theory to phononic scattering in a three-dimensional crystal, both as unit cell and superlattice configuration, where boundary scattering is present.

Herbold and Nesterenko [144] worked on the rarefaction pulses that take place in discrete materials with a strain-softening behaviour, which can be categorised as solitary waves. They could be helpfully employed in destruction of acoustic and shock waves. Ganesh and Gonella [145] developed a framework for spatial and modal wave manipulation in nonlinear granular crystals with a range of topologies, in order to obtain wave control functionalities and program the response. Instabilities are another nonlinear phenomenon which affects dynamical response of metamaterial devices. Nadkarni et al. [146] studied transition waves in a periodic lattice of bistable elements with magnetic connections. The bistability of the elements induce asymmetry in the energy wells and thus unidirectional transitions, enabling the realization of waveguides and energy harvesters. Likewise, Raney et al. [147] investigated signal propagation in soft bistable structures, with the goal of avoiding dissipation of mechanical signals due to the nature of flexible materials. Nonlinear solitary waves transmission is obtained through a specific architecture.

In their work from 2021 [148], Settini et al. examine the nonlinear response that insurges from a 1D cellular lattice with a indeformable pantograph mechanism. Hardening and softening behaviours are observed. This was also observed by Manimala et al. [149], who investigated the amplitude-dependent dynamic response in acoustic metamaterials. The bandgaps shifts due to both hardening and softening nonlinearities are investigated, offering further opportunities for dispersion relation tuning.

Fronk and Leamy [150] expanded the analysis of weakly nonlinear chains through perturbation methods to higher orders. In most of the previous publications on weak nonlinearity a cubic stiffness is considered, as it seems to be influencing dispersion relation shifts in a more considerable way compared to quadratic stiffness. However, as shown in this study, when considering higher perturbation orders in multiple scales analysis both cubic and quadratic stiffnesses result in dispersion correction terms, where the quadratic terms could provide an useful tool for generating travelling, invariant plane waves to transmit information.

From an experimental point of view, Parmley et al. [151] studied the dispersion properties of a nonlinear string-mass chain, both finding the theoretically predicted eigenmodes and Anderson localization modes. Furthermore, Zega et al. [152] experimentally studied the phenomenon of subharmonic attenuation zones in nonlinear locally resonant metamaterials.

Strong nonlinearities, on the other hand, are hardly solved through analytical approaches, and the numerical solutions can present bifurcations and instability.

In a study from 2016, Fang et al. [153] investigated the tunability properties of a one-dimensional chain with locally resonant masses, tied to the main system through nonlinear couplings. Rushchitsky et al. [123] analysed the role of material nonlinearities in longitudinal and transverse wave propagation, by considering a constitutive material with a Murnaghan potential. It is shown that frequencies can switch to different bands due to energy transfer, which could constitute an useful tool in designing mechanical circuits for wave manipulation.

In order to account for strong nonlinearities in periodic systems, Narisetti et al. [154] implemented strong nonlinearities into a discrete 1D and 2D lattice model. The proposed method is an extension of the Harmonic Balance Method (HBM) to a periodic system, thus accounting for Bloch-Floquet boundary conditions. The nonlinearity is implemented through Hertzian contact between the beads. Amplitude dependent behaviour is detected in the dispersion curves and the solution shows multiple frequency and wavenumber components for each unit cell.

The dynamic response yielded from impacts was also investigated by Yang et al. [155], who studied wave propagation in a chain of particles along elastic guides under the impact of an external mass. The propagation of forces and compression waves along the system is investigated, with attention to the interplay between the granular particles and the elastic medium, both numerically and experimentally. The deflection of the elastic guides and the corresponding energy are shown to be tunable through the initial curvature of the chain, and the same applies to the propagation of impacts.

For tuning purposes, Medina et al. [156] investigated a framework to design flexible mechanical metamaterials to achieve targeted responses under specific loadings. The study highlights the opportunities of using aperiodic lattices when dealing with nonlinear constitutive materials, as shape optimization algorithms show that targeted behaviours are often found in atypical domains.

4.1.4 Chaos in periodic discrete systems and metamaterials

The chaos theory is concerned with dynamical systems that, even though they are governed by deterministic laws, exhibit an erratic and unpredictable behaviour in the long term [130]. Chaotic behaviour is generally associated with nonlinear systems. Understanding it -to the extent to which this is possible- is paramount, as it is present in several natural and artificial systems, and in the engineering field to design solid devices and technologies which are not subject to drastic unpredictabilities. This apparently paradoxical phenomenon is due to extreme sensitivity to initial conditions. In many dynamical systems subject to chaos, the trajectories of the system in the phase space form the so called strange attractors. An attractor represents a set of states towards which a system tends to evolve, depicted in the phase space. A strange attractor is locally unstable, as, depending on the initial conditions, two close-by states can arbitrarily develop to states far away from each other. .

In mechanical metamaterials, nonlinearity is generally found according to intentional design choice, in order to reach certain responses in the static and dynamic range. Among others, it can be useful

to enhance vibration amplitudes for energy harvesting purposes or to localise waves and hinder the diffusion, for instance for damping and absorption. However, the insurgence of chaotic responses can hinder the attainment of those scopes. In dynamics, this leads to erratic, i.e. aperiodic, responses to harmonic excitation, with unpredictable shifts in frequency and amplitude. Furthermore, a back and forth transition from chaotic behaviour can be abrupt.

The mathematical treatment of chaotic behaviour usually involves Poincaré maps, which show the velocity versus the displacement of points in the system for every timestep or iteration, to observe its evolution. Another technique involves the usage of Lyapunov exponents, which measure the velocity with which the trajectories of a system get farther from one another, in order to evaluate the sensitivity to initial conditions. Power density spectra are further tools which can be employed to visualize the distribution of energy among the different frequencies of the systems. All in all, the study of chaotically behaving systems generally involve numerical calculations as the responses can not be determined analytically.

In the thorough work by Shi et al. [157] the insurgence of chaos in periodic systems is studied, and some criteria are laid out in order to avoid it. Fang et al. [158] exploited the chaotic behaviour of one-dimensional and two-dimensional nonlinear acoustic metamaterials to enhance bandgaps and reduce noise propagation. On the other hand, Al Ba'ba'a et al. [159] studied the impact of undesired, manufacturing-caused nonlinearities onto metamaterials' dynamic response. As mentioned earlier, the behaviour of metamaterials, that have properties which depend on their subwavelength periodic structure, is easily hindered by imperfections or constitutive materials' properties. When the finite structures are assembled and tested, their response to dynamic excitations does not necessarily correspond to the envisioned one, the band gaps could be shifted with respect to the design ones, referring to the infinite chain, and the response often can lean to anharmonic oscillations (chaotic, erratic ones). Their analysis focuses on the quantification of these uncertainties through polynomial chaos, in order to obtain confidence levels to guide the design process for targeted performances. Fang et al. [160] apply the homotopy analysis method to derive dispersion characteristics of nonlinear multi-atomic chains, and compare the results to more commonly employed methods as the harmonic balance method and perturbation methods, in this way highlighting how strong nonlinearities are beneficial to low-frequency bandgaps.

4.1.5 The role of BNN connections in nonlinear metamaterial design

The coupling between nonlocality and nonlinearity was explored in the phononic crystals field by Henstridge et al. [161], demonstrating that the addition of nonlinearity and anharmonic oscillations can be helpful in controlling the functional properties of complex solids. In fact, as mentioned above, the framework for dynamic systems, the presence of nonlinearity in different forms (material, geometric, from contact and so on) can enhance the response of the excited system due to generations of super- or sub-harmonics. This could be helpfully employed in metamaterial design to achieve shifts in frequency spectra, tied to the amplitude dependency of the dispersion curves.

With reference to the topic of BNN connections in periodic lattices in the field of elastic metamaterial design, and the roton-like behaviour these devices own, in this chapter follow-up note to the recent paper by the author and coworkers on *mechanical consistency* in nonlocal lattice models [120] is presented, where an overall mass conservation law is enforced in order to establish a clear ratio between the mass of the beads and of the links. This ensures that the hypothesis of the springs' masses not contributing to the dynamics of the system, normally employed in harmonic oscillation models, is abided by, regardless of the number of nonlocal connections. The work presented here considers the case of weak nonlinearity due to a nonlinear restoring force law, following a perturbation approach. ([124], [126], [30]). The nonlinearity is expressed through a cubic law, however multiple approaches could be equally employed [121]. A mass conservation criterium is applied to the nonlinear component of the springs' stiffnesses, and the tuning parameters previously proposed,

the stiffness distribution parameter α and the P level of nonlocality are made available for nonlinear systems. Dispersion curves for the mass-conserving nonlocal and nonlinear case are retrieved, and the amplitude-dependency of the resonance frequencies can be observed. Numerical validation through explicit dynamics simulations follows.

4.2 Modelling and analysis

The model considered is a monoatomic chain with N elements connected to each other with longitudinal springs. The system is periodic and obeys the Bloch-Floquet boundary conditions, with the system being generated by an array of unit cells with length a . The nonlocality level P rules over the number of connections that the unit cell has to its adjacent elements.

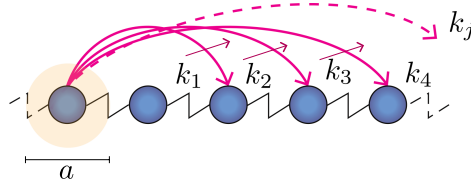


Figure 4.1: Scheme of the periodic nonlocal 1D mass spring chain. The highlighted area represents the unit cell, of length a , with its P number of connections with stiffness $k_1, k_2 \dots k_j$ to the other unit cells at distance ja , i.e. at a distance directly proportional to the nonlocality level, which feature the same connections to the neighbours. Every link, both local and nonlocal, contains a linear and a weakly nonlinear component.

As mentioned in Section 1, a nonlinear restoring force is added to the springs in the system, so that for each spring converging in the unit cell

$$k_{j,nl}^{(P)} = k_{0,j}^{(P)} f(x), \quad (4.1)$$

where $k_{0,j}^{(P)}$ is the linear elastic component to the spring's stiffness, the subscript j refers to the level of nonlocality associated to the spring considered, the superscript (P) to the level of nonlocality of the chain, and $f(x)$ is a function of displacement, which will depend on the nonlinear constitutive law considered, as the Neo-Hookean or Mooney Rivlin. As long as the function representing displacement is continuous and derivable (C^∞), it can be expanded in series and thus approximated through a polynomial function as $F(x)$ with

$$\begin{aligned} f(x) &= 1 + \beta x + \gamma x^2 + o(x^3) \\ F(x) &= 1 + \beta x + \gamma x^2. \end{aligned} \quad (4.2)$$

In this case, springs composed by a linear and a cubic component will be considered, thus it will be assumed that $\beta = 0$.

4.2.1 Volume conservation hypothesis

The deformation of nonlinear elastic elements, supposed isotropic and homogeneous, can be described through a deformation gradient $\mathbf{F}$ defined as follows,

$$\mathbf{F} = \mathbf{I} + \nabla \mathbf{x}. \quad (4.3)$$

It is thus assumed that the deformation gradient has a diagonal form, namely

$$\mathbf{F} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \quad (4.4)$$

where $\lambda_i = l_i/L_i$ is the stretch and $i \in [1, 2, 3]$.

From 4.3,

$$\begin{aligned} \lambda_1 &= 1 + \frac{\partial x}{\partial x_1} \\ \lambda_2 &= 1 + \frac{\partial x}{\partial x_2} \\ \lambda_3 &= 1 + \frac{\partial x}{\partial x_3} \end{aligned} \quad (4.5)$$

where, in the specific case of circular section, $\lambda_2 = \lambda_3 = \lambda_T$ becomes the transversal component, and $\lambda_1 = \lambda_L$ for the longitudinal one.

By definition, $\det \mathbf{F} > 0$, and

$$\det \mathbf{F} = \lambda_L \lambda_T^2 \quad (4.6)$$

which becomes, in the isochoric case

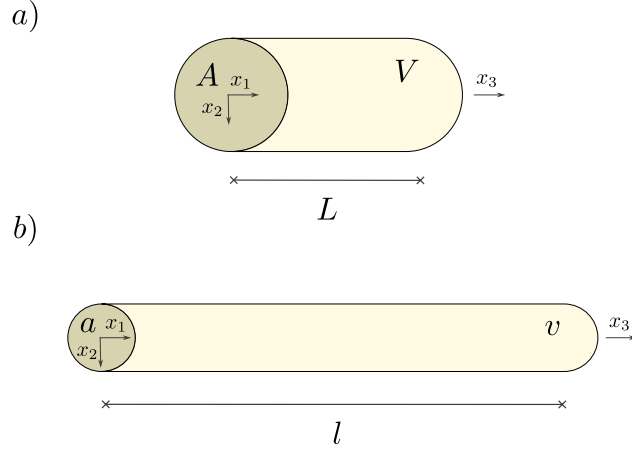


Figure 4.2: Scheme of a spring of whichever nonlocality level $j \in [1, \dots, P]$, with a circular section. When the element is stretched beyond the linear limit, the constant density hypothesis is not abided by and $v \neq V$, unless there is an isochoric restriction, i.e. $V = v = \text{const}$

$$\det \mathbf{F} = 1, \quad \lambda_L \lambda_T^2 = 1 \implies \lambda_T^2 = \lambda_L^{-1} \quad (4.7)$$

In the general case the initial volume will differ from the final one due to a variation in density of the material, but the mass will remain unvaried

$$\rho dv = \rho_0 dV \quad (4.8)$$

where $dv = JdV$ and $J = \det \mathbf{F}$ Jacobian. In the isochoric case, by plugging in equation 4.6 for the determinant

$$\begin{aligned}\rho\lambda_T^2\lambda_L dV &= \rho_0 dV \\ \rho &= \rho_0\lambda_T^{-2}\lambda_L^{-1}\end{aligned}\tag{4.9}$$

gives the expression for the updated density value ρ .

Given this first overview on nonlinear elasticity, the *mechanical consistency* condition is enforced on nonlinear springs through the mass itself rather than the volume, as the density ρ_0 can not always be regarded as constant.

In the isochoric case $v = V$ and equations 2.10, 2.14 hold true.

On the other hand, when the volume is not conserved, the *mechanical consistency* condition on the unit cell will be

$$\mu = \frac{m_s}{m} = \frac{\rho_0 V}{m} = \frac{\rho v}{m} \ll 1\tag{4.10}$$

where m represents the mass of the atom in the unit cell and m_s the total mass of the springs, given respectively by $\rho_0 V$ and ρv in the initial and final phases of the deformation.

The mass m_s can be expressed consequently as

$$m_s = \sum_{j=1}^P A_{j,nl}^{(P)} jL\rho_0 = \sum_{j=1}^P a_{j,nl}^{(P)} jl\rho\tag{4.11}$$

with $A_{j,nl}^{(P)}$ initial cross-section and jL initial length of the j^{th} level of nonlocality spring, and $a_{j,nl}^{(P)}$ and jl their final values.

The springs are considered to be uniaxial, therefore the stiffness constant $k_{0,j}^{(P)}$ in 4.1 is expressed as $k_{0,j}^{(P)} = \frac{EA_j^{(P)}}{jL}$. The equations derived in Chapter 2 will be thus valid to apply mass conservation to nonlinear springs, as the constraint is imposed to the cross-sections of the links and the material density is assumed as constant, and the length as directly proportional to the nonlocality level of the connection. As the nonlinearity is assumed to be weak, a fraction of the mass of the linear springs is assumed as constant volume for the nonlinear ones $m_{s,nl} = \epsilon m_{const}$, with a small parameter ϵ to tune the strength of the nonlinearity. The equations, considering equation 4.11, will then read

$$\sum_{j=1}^P A_{nl,j}^{(P)} ja\rho_0 = \epsilon m_{const} = m_{nl},\tag{4.12}$$

or

$$\sum_{j=1}^P A_{nl,j}^{(P)} ja = \epsilon \frac{m_{const}}{\rho_0} = \bar{m}_{const},\tag{4.13}$$

The mass balance, as in the previous part, presents a P number of unknowns, the cross sections, and can be solved only through establishing a relation between them. It is here assumed

$$A_{nl,j}^{(P)} = \frac{A_{nl,1}^{(P)}}{j^{\alpha_{nl}}},\tag{4.14}$$

with α_{nl} being the *stiffness distribution parameter* for the nonlinear connections. The mass balance equation yields for every case of P and α_{nl} values:

$$A_{nl,1}^{(P)} = \frac{1}{\sum_{j=1}^P j^{1-\alpha_{nl}}},\tag{4.15}$$

The $f(u)$ considered has a linear and a cubic term, namely:

$$f(x) = k_0(1 + \gamma x^2), \quad (4.16)$$

By simplifying to $\alpha = \alpha_{nl}$, and $E = E_{nl}$, from the initial assumption $m_{s,nl} = \epsilon m_s$:

$$\gamma = \epsilon = \frac{A_{nl,j}^{(P)}}{A_j^{(P)}}, \quad (4.17)$$

Thus, from 2.14 and $k_0 = k_j^{(P)}$, and 4.1,

$$k_j^{(P)} = \frac{EA_j^{(P)}}{ja}, \quad (4.18)$$

where E is the Young modulus of the raw spring material, ja is the length of the j^{th} link considering its unit length corresponding to that of the unit cell $L = a$, without loss of generality, and $A_j^{(P)}$ is the corresponding cross section, in which the subscript indicates it connects the j^{th} next neighbour and the superscript denotes the maximum number of BNN connections in the designed chain.

4.2.2 Perturbation approach

As the nonlinearity considered is weak, i.e., the magnitude of the stiffness of the nonlinear springs is considerably lower than that of the linear springs, perturbation methods can be applied to retrieve the harmonic behaviour.

The equation of motion for the nonlinear and nonlocal system, neglecting viscous contributions, thus reads:

$$m\ddot{x}_n + \sum_{j=1}^P k_{0,j}^{(P)}(2u_n - x_{n-j} - x_{n+j}) + \sum_{j=1}^P k_{j,nl}^{(P)}[(x_n - x_{n-j})^3 + (x_n - x_{n+j})^3] = 0, \quad (4.19)$$

where $k_{j,nl}^{(P)} = \epsilon k_{0,j}^{(P)}$, and $\epsilon = \frac{A_{nl,j}^{(P)}}{A_j^{(P)}} \ll 1$.

4.2.3 Linstedt-Poincaré asymptotic expansion

The equation 4.19 above can be solved semi-analytically through a perturbation technique, namely the Linstedt-Poincaré asymptotic expansion. In order to do so, a perturbation parameter is identified in ϵ , small in comparison to the other quantities of the problem.

The problem is rewritten through the dimensionless variable τ and the normalization frequency ω_n below

$$\tau = \omega t, \quad \omega_n \propto \sqrt{\frac{\sum f(k_i)}{m}} \quad (4.20)$$

Plugging the dimensionless time into the equation and dividing everything by $m\omega_n^2$ yields:

$$\bar{\omega}^2 \frac{d^2 x_n}{d\tau^2} + \sum_{j=1}^P \bar{k}_{0,j}^{(P)}(2x_n - x_{n-j} - x_{n+j}) + \epsilon \left(\sum_{j=1}^P \bar{k}_{j,nl}^{(P)}[(x_n - x_{n-j})^3 + (x_n - x_{n+j})^3] \right) = 0 \quad (4.21)$$

where $\bar{k}_j^{(P)} = k_j^{(P)} / (m\omega_n)$.

The solution can be expressed through the first terms of an asymptotic expansion, which becomes more accurate as the limit $\epsilon \rightarrow 0$ approaches. The variables are thus approximated as

$$\begin{aligned} x_n &= x_n^{(0)} + \epsilon x_n^{(1)} + O(\epsilon^2) \\ \omega &= \omega_0 + \epsilon \omega_1 + O(\epsilon^2), \end{aligned} \quad (4.22)$$

with ϵ being the aforementioned small parameter.

Inserting the approximated variables into the

$$\begin{aligned} \frac{d^2 x_n^{(0)}}{d\tau^2} + \epsilon(\bar{\omega}_0^2 \frac{d^2 x_n^{(1)}}{d\tau^2} + 2\bar{\omega}_0 \bar{\omega}_1 \frac{d^2 x_n^{(0)}}{d\tau^2}) &= - \sum_{j=1}^P \bar{k}_j (2x_n^{(0)} - x_{n-j}^{(0)} - x_{n+j}^{(0)}) + \\ - \epsilon \left(\sum_{j=1}^P \bar{k}_j (2x_n^{(1)} - x_{n-j}^{(1)} - x_{n+j}^{(1)}) \right) &+ \sum_{j=1}^P \bar{k}_j^{(P)} ((x_n^{(0)} - x_{n+j}^{(0)})^3 + (x_n^{(0)} - x_{n-j}^{(0)})^3) \end{aligned} \quad (4.23)$$

The terms of the equation are separated according to their order of magnitude, therefore at the 0^{th} order a unforced, undamped linear

$$\frac{d^2 x_n^{(0)}}{d\tau^2} - \sum_{j=1}^P \bar{k}_j^{(P)} (2x_n^{(0)} - x_{n-j}^{(0)} - x_{n+j}^{(0)}) = 0, \quad (4.24)$$

where the superscript (0) refers to the order of magnitude of the solution. This problem has a known solution, that is

$$\begin{aligned} x_n^{(0)} &= \frac{\Omega_1^{(0)}}{2} e^{ikna} e^{i\tau} + \frac{\bar{\Omega}_1^{(0)}}{2} e^{-ikna} e^{-i\tau} \\ x_{n\pm j}^{(0)} &= \frac{\Omega_1^{(0)}}{2} e^{ika(n\pm j)} e^{i\tau} + \frac{\bar{\Omega}_1^{(0)}}{2} e^{-ika(n\pm j)} e^{-i\tau} \end{aligned} \quad (4.25)$$

where $\Omega_1^{(0)}$ is the amplitude of the driving force, and $\bar{\Omega}_1^{(0)}$ its complex conjugate. The 0^{th} order resonance frequencies are obtained as

$$\bar{\omega}_0 = \sqrt{2 \left(\sum_{j=1}^P \bar{k}_{0,j}^{(P)} (1 - \cos(j\kappa a)) \right)} \quad (4.26)$$

which corresponds to the classical linear, nonlocal dispersion relation.

The perturbation to the solution given by the nonlinearity is to be retrieved at higher orders, as the nonlinear terms are included in the 1^{st} . The second equation, for order ϵ_1 , reads:

$$\begin{aligned} \bar{\omega}_0^2 \frac{d^2 x_n^{(1)}}{d\tau^2} + \sum_{j=1}^P \bar{k}_{0,j}^{(P)} (2x_n^{(1)} - x_{n-j}^{(1)} - x_{n+j}^{(1)}) &= -2\bar{\omega}_0 \bar{\omega}_1 \frac{d^2 x_n^{(0)}}{d\tau^2} + \\ - \sum_{j=1}^P \bar{k}_{0,j}^{(P)} (2x_n^{(1)} - x_{n-j}^{(1)} - x_{n+j}^{(1)}) &- \sum_{j=1}^P \bar{k}_j^{(P)} ((x_n^{(0)} - x_{n+j}^{(0)})^3 + (x_n^{(0)} - x_{n-j}^{(0)})^3) \end{aligned} \quad (4.27)$$

which can be regarded as a generalised harmonic oscillator problem with forcing, which is given by the $u^{(0)}$ terms previously retrieved. The driving force has both natural frequencies and M multiples

of its value, depending on the restoring law considered, therefore secular terms will emerge from the former. From the superposition of the solution for the undriven oscillator and the forced oscillator, the overall solution will be

$$x_n^{(1)}(\tau) = a_1 \sin(\tau) + \sum_{m=2}^M b_1 \sin(m\tau) + c_1 \tau \sin(\tau), \quad (4.28)$$

where the last term is unbounded, as it is a secular term and must be suppressed for an oscillatory solution.

By solving the differential problem in equation 4.27 and imposing $c_1 = 0$ for the coefficient of the secular term, the correction to the linear dispersion curve is then retrieved by solving the equation at the 1st order of ϵ as

$$\bar{\omega}_1 = \frac{3|\Omega_1^{(0)}|^2 (\sum_{j=1}^P -\bar{k}_{0,j}^{(P)} + 4\bar{k}_{0,j}^{(P)} \cos(j\kappa a) - \bar{k}_{0,j}^{(P)} \cos(2j\kappa a))}{4\bar{\omega}_0}, \quad (4.29)$$

which can be simplified through trigonometric relations as

$$\bar{\omega}_1 = \frac{3|\Omega_1^{(0)}|^2}{8} \bar{\omega}_0^3. \quad (4.30)$$

The overall dispersion relation, as for the asymptotic expansion, is thus

$$\bar{\omega} = \bar{\omega}_0 + \epsilon \bar{\omega}_1, \quad (4.31)$$

which features a dependency both on the magnitude of the nonlinear contribution given by the value of ϵ and from the amplitude of the driving force, as Ω_1 appears in the frequency correction.

4.2.4 Multiple scales method

An alternative path that leads to the perturbed dispersion curves, is the Multiple Scales method, as presented in [128] and applied to periodic systems in [126]. This method is usually applied to problems where there are regions of non-uniformity of the straightforward expansion in the subsection above, due to either an infinite domain or the occurrence of singularity. These problems are amended by recognising the existence of more than one temporal or spatial scale, in this case the first as follows:

$$t \rightarrow t, T_1, T_2, T_3 \dots f(t) \rightarrow f(t, T_1, T_2, T_3 \dots). \quad (4.32)$$

Then, the solution is assumed in the form of a general asymptotic expansion:

$$f(t, \epsilon) = \sum_m f_m(t, T_1, T_2, T_3, \dots) \epsilon^m, \quad \epsilon \rightarrow 0 \quad (4.33)$$

Thereafter, this is substituted into the differential problem and solved at the various orders of approximation in the perturbation parameter ϵ , in terms of $t, T_1, T_2, T_3 \dots$, using the following chain rule:

$$\frac{d}{dt} \rightarrow \frac{\partial}{\partial t} + \epsilon^m \frac{\partial}{\partial T_m} \quad (4.34)$$

and the secular terms are suppressed by imposing boundary conditions.

4.3 Explicit numerical simulations through Runge-Kutta method

As the results can vary widely when considering a weakly nonlinear analytical solution and a strongly nonlinear system, the results obtained from the methods presented above are then compared to the results of direct numerical simulations. As the system at hand is nonlinear, the matrix-based Newmark method can not be employed anymore, therefore the numerical simulations are ran through the Runge Kutta method.

4.3.1 Runge Kutta method for nonlinear dynamics of a multidof system, an overview

Consider a second-order Ordinary Differential Equation of the form

$$\frac{\partial^2 x}{\partial t^2} = f\left(t, x, \frac{\partial x}{\partial t}\right) \quad (4.35)$$

To apply the RK4 method, which only deals with first order ODEs, equation 4.35 can be decomposed into a system of two first-order ordinary differential equations. First, a new variable x' is defined for the temporal derivative of x :

$$x' := \frac{\partial x}{\partial t} \quad (4.36)$$

then, rewrite equation is rewritten as

$$\begin{cases} \frac{\partial x'}{\partial t} = f(t, x, x') \\ \frac{\partial x}{\partial t} = g(t, x, x'), \quad g(t, x, x') = x' \end{cases} \quad (4.37)$$

Then the RK4 can be employed, using its capability to deal with function of multiple variables. First the coefficients k_i and j_i are computed, which correspond to the first and second equation of system 4.37, respectively:

$$\begin{aligned} k_1 &= f(t_n, x_n, x'_n) \\ j_1 &= g(t_n, x_n, x'_n) \\ k_2 &= f\left(t_n + \frac{\Delta t}{2}, x_n + \frac{\Delta t}{2}k_1, x'_n + \frac{\Delta t}{2}j_1\right) \\ j_2 &= g\left(t_n + \frac{\Delta t}{2}, x_n + \frac{\Delta t}{2}k_1, x'_n + \frac{\Delta t}{2}j_1\right) \\ k_3 &= f\left(t_n + \frac{\Delta t}{2}, x_n + \frac{\Delta t}{2}k_2, x'_n + \frac{\Delta t}{2}j_2\right) \\ j_3 &= g\left(t_n + \frac{\Delta t}{2}, x_n + \frac{\Delta t}{2}k_2, x'_n + \frac{\Delta t}{2}j_2\right) \\ k_4 &= f(t_n + \Delta t, x_n + \Delta t k_3, x'_n + \Delta t j_3) \\ j_4 &= g(t_n + \Delta t, x_n + \Delta t k_3, x'_n + \Delta t j_3) \end{aligned} \quad (4.38)$$

The values of the dependent variables (i.e. unknowns) x and x' at the subsequent time step $n + 1$ are then computed:

$$\begin{aligned} x_{n+1} &= x_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\ x'_{n+1} &= x'_n + \frac{1}{6}(j_1 + 2j_2 + 2j_3 + j_4). \end{aligned} \quad (4.39)$$

4.4 Results and discussion

In the nonlinear case, the dynamic behaviour of the chains is amplitude dependent. Therefore the dispersion curves shift in frequency as the amplitude of the excitation changes. In Figure 4.3, this effect is shown for two different levels of nonlocality P , which retain their typical local minima and maxima while shifting in the frequency range.

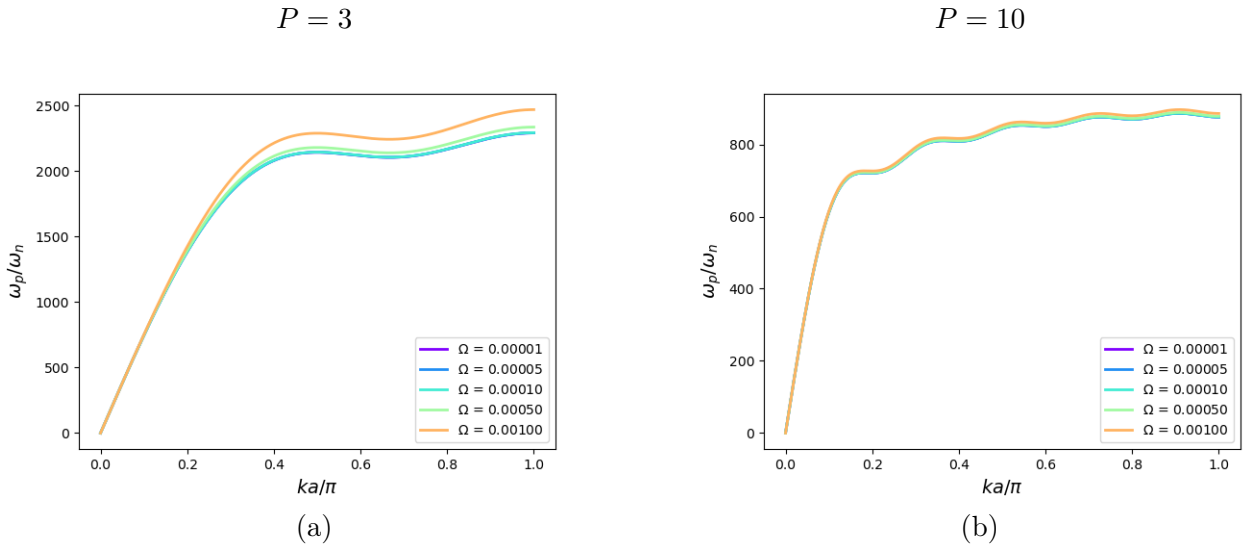


Figure 4.3: In the Figure the dispersion relations for $\alpha = 0$ and $\epsilon = 0.01$ are shown for (a) $P = 3$ and (b) $P = 10$. The variation in amplitude, $\Omega[m]$, causes the frequency spectrum to shift, while maintaining the behaviour, i.e., the number of local minima and maxima due to BNN connections.

Figure 4.3 illustrates the amplitude-dependent frequency shifts in the dispersion relation of the weakly nonlinear mass-conserving monoatomic chain, due to varying Ω values. Figure 4.3 (a) and (b) respectively show the dispersion relations for $P = 3$ and $P = 10$, both with a stiffness distribution parameter $\alpha = 0$ and the small parameter controlling the nonlinearity level $\epsilon = 0.01$.

In both subfigures 4.3 (a) and (b), the variation in amplitude Ω , causes the dispersion curves to shift in frequency, while maintaining the number of local maxima and minima proportional to the level of nonlocality P , i.e. three in (a) and ten in (b). The fundamental wave propagation properties of the model are thus unbothered by the weak nonlinearity, as expected from literature ([124], [126], [30]).

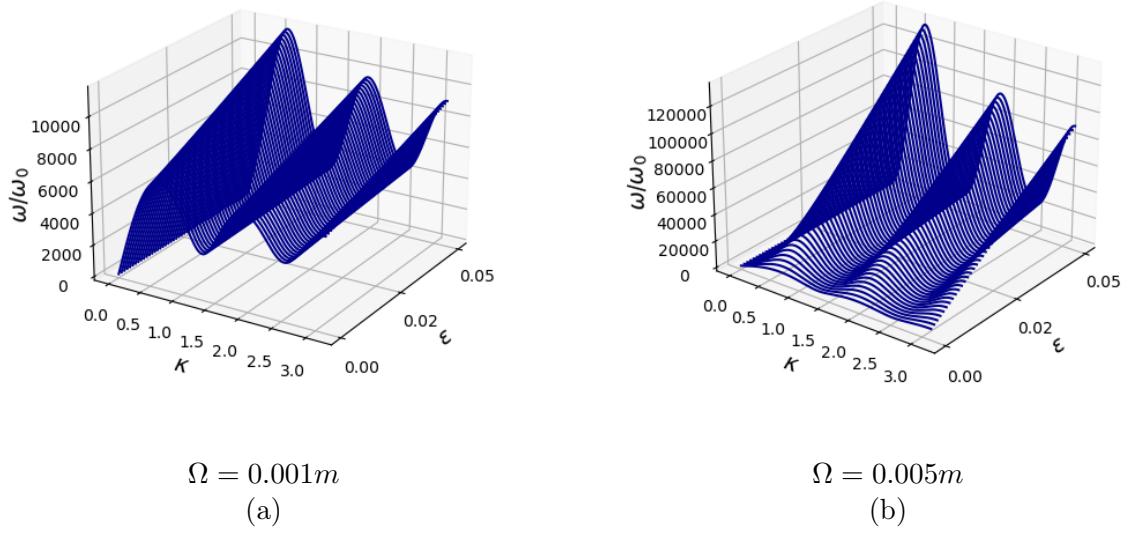


Figure 4.4: In the Figure a 3D graph of the dispersion relations ($\omega - \kappa$ planes) are displayed for several levels of nonlinearity, i.e. ϵ values. In these cases $\alpha = 0$ and $P = 5$, and in (a) $\Omega = 0.001m$, in (b) $\Omega = 0.005m$. In (a), with a smaller perturbation amplitude, the resulting dispersion curves are not shifting in value with the choice of the small parameter ϵ , while when the amplitude of the forcing is larger the frequency value is highly dependent on the level of nonlinearity.

Figure 4.4 illustrates the amplitude-dependent dynamic behaviour of the studied metamaterial chains, and the impact of varying the degree of nonlinearity on the system's dispersion relations. It presents two 3D graphs, (a) and (b), showing the dispersion relations ($\omega - \kappa$ planes) for different levels of nonlinearity and response amplitude (respectively ϵ and Ω values). The values of the stiffness distribution parameter is $\alpha = 0$, and the non-locality level $P = 5$ in both sub-figures

The most significant observation from Figure 4.4 is that the dynamic behaviour of the chain is highly dependent on the amplitude of the excitation. In fact, the difference in the dynamic behaviour attained from models with a shift in the amplitude of the forcing can be observed. In Figure 4.4 (a), where the excitation amplitude is small ($\omega = 0.001m$), the resulting dispersion curves do not significantly shift in value with changes in the small parameter ϵ . This indicates that when the excitation amplitude is under a certain threshold, the amplitude shifts induced by the nonlinearities have less impact on the frequency range of the dispersion curves. However, in Figure 4.4 (b), where the excitation amplitude is larger ($\omega = 0.005m$), the frequency values become highly dependent on the level of nonlinearity (ϵ). The strong amplitude-dependent behaviour demonstrates the potential for creating tunable devices. By adjusting the excitation amplitude and the level of nonlinearity (ϵ), the frequency response of the system can be potentially significantly shifted. The results of this approximated method, however, heavily rely on the nonlinearity being weak to be able to retrieve a realistic result, which should be numerically validated case by case.

4.4.1 Numerical validation

In this section, the numerical validation of the perturbation analysis results is carried out through the *Runge Kutta 4* integration method, which is chosen for this problem due to the nonlinear components.

Nonlocal models present some limitations, as they require an infinite number of elements to fully achieve the desired level of nonlocality. In a discrete system, it is essential that the ratio of the nonlocality level P to the number of masses N remains below a certain threshold. This ensures that

the bulk of the chain dominates the dynamic behaviour, as the $2P$ boundary masses at the ends of the chain are only connected to their beyond-nearest neighbours on one side, while being fixed on the other.

To balance computational efficiency and boundary effects, a chain consisting of 1000 masses with fixed ends is used in the simulations.

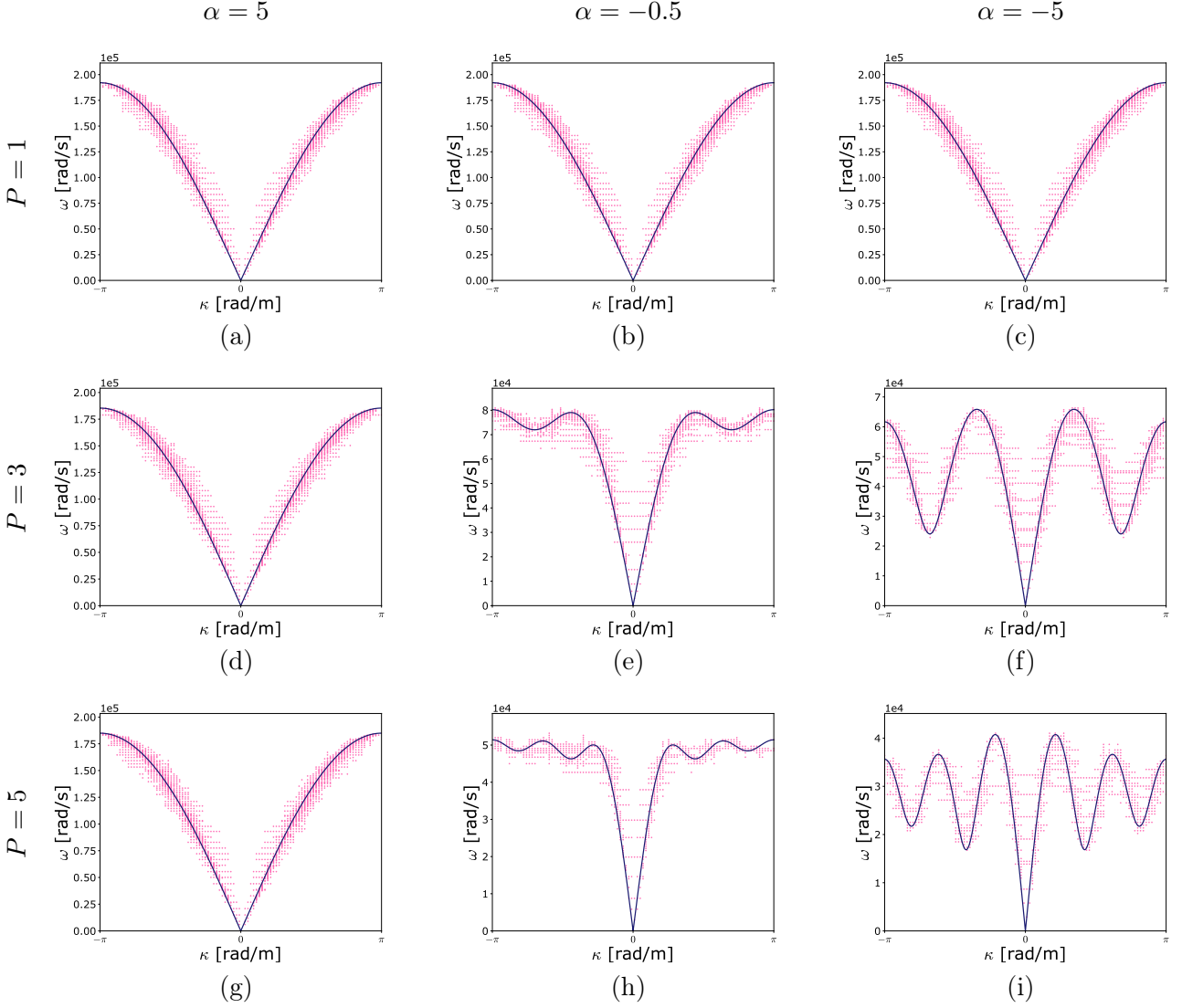


Figure 4.5: The Figure above shows the comparison between the numerical solution (in pink) and the perturbative one (blue). The amplitude considered in both the perturbative solution and the chirp modulation forcing is $\Omega = 0.005 m$, while $\epsilon = 0.001$ for the nonlinear springs' mass calculation as $m_{s,nl} = \epsilon m_s$, therefore $\mu = \epsilon \mu$. The 2D FFTs reproduce the behaviour of the analytical predictions in the finite case, with the curves being monotonic or not corresponding to the nonlocality level P and α values.

The results were obtained from numerical simulations conducted in Python using *Runge Kutta 4* integration method, as mentioned above. Initial conditions were set as $\ddot{u}_n = 0$, $\dot{u}_n = 0$, and $u_n = 0$, meaning no initial acceleration, velocity, or displacement were applied to any of the masses. The system is excited using a time-varying force applied on the central mass, with a chirp modulation to excite the system across a range of frequencies, thus enabling the construction of the dispersion curves by capturing the system's response to various eigenfrequencies.

The time-domain explicit dynamics results were finally processed via a 2D Fast Fourier Transform to obtain the frequency-domain data, representing the dispersion curves for the finite chain.

For a small value of both the excitation amplitude Ω and of the perturbation parameter ϵ , the simulation results are in good agreement with the analytical model.

Figure 4.5 illustrates the numerical validation of the perturbative solutions obtained for the system by comparing them with the results of explicit numerical simulations. The nine subplots refer to different α, P combinations, while the values of ϵ and Ω are kept constant, each showing the overlay of perturbative solutions (in blue) on top of the numerical results (in pink).

The results demonstrate that by carefully designing non-local interactions and introducing weak cubic nonlinearities, wave propagation characteristics can be controlled through frequency shifts, offering new possibilities for the design of advanced metamaterials. A key feature of this study is the implementation of a mass conservation law, which ensures *mechanical consistency* allows for comparisons between local and non-local lattices. This is critical for ensuring that the mass of the springs does not contribute to the system's dynamics, which is commonly neglected in discrete harmonic oscillation models. By extending this law to nonlinear couplings, the model simplifies the design process for metamaterials with specific properties and provides two parameters to control the desired outcome, the stiffness distribution parameter α and the nonlocality level P .

The study is built upon the work of Narisetti et al. [124] and Manktelow et al. [126], both of whom used perturbation methods to analyse wave propagation in nonlinear systems. However, this study incorporates non-local interactions and introduces a reasoning on mass constraints in nonlocal models, while the above-mentioned works focused on local systems with weak nonlinearities. Non-local interactions allow for greater flexibility in tailoring dispersion characteristics, as enabling negative group velocities and backwards propagating energy.

Cubic nonlinearities are used to model the restoring force in the system in both this work and the reference ones. This choice of nonlinearity is motivated by its significant impact on the system's dispersion characteristics. Cubic nonlinearity, in fact, modifies the dispersion curves from the first order of approximation in the perturbation procedure, creating superharmonics which would not be present by considering quadratic ones. Monoatomic chains are used in all studies as a model system, simplifying the analysis while still capturing essential wave propagation effects. This approach allows for a more manageable framework to study the complex dynamics of nonlinear systems.

4.5 Conclusions

This study explored the combined effects of non-locality and nonlinearity in one-dimensional monoatomic chains, building on the previously proposed *mechanical consistency* condition for elastic connections and expanding to weak nonlinearities. The work shown here discusses the presence of weakly nonlinear springs in the context of nonlocal connections in mass-conserving monoatomic chains. The *mechanical consistency* condition previously proposed by the authors is extended to nonlinear media. Nonlinearity is inherent in real-models and its addition is necessary when the levels of complexity of engineering devices grows and some nonlinear components could be present. In fact, in envisaging wave filtering devices, the goal is to be able to predict which frequencies will make contact with the object and how will it behave. A certain amount of nonlinearity in the predictive models not only ensures a more accurate dynamical response, but provides a further degree of freedom in the tuning capabilities as well. The amplitude-dependent frequency shifts allow for larger dispersion spectra to be attained from the very same amount of material. Frequency mixing and solitons are additional effects that could be achieved, among others, for wave guides for instance. A step further in this analysis would include strong nonlinearities and their effect on periodic systems. The dynamical response of such systems is not necessarily harmonic, instead, it could be, as a matter of fact, chaotic. In order to avoid any undesired, unpredictable effect, developing effective measures of chaos estimate and control would be

beneficial to the employment of nonlinear properties in metamaterials. A second possible extension to this concept would include mass conservation criteria for springs' with material, i.e., constitutive nonlinearities, which are far more common in the real world. Overall the authors reckon that the expansion of the proposed mass-conservation model to a broader class of dynamic systems could be helpfully employed to make sure that modelling nonlocal connections does not contradict the hypotheses of the equations used in the analyses. Moreover, the design of several prototypes from the very amount of mass will lead to reasonable dynamic response comparisons and to a better insight of the weights of the contributions of the components of the imagined designs.

Chapter 5

Generalising mass-conservation to two-dimensional nonlocal lattices

Abstract

Metamaterials, artificial lattices with dynamical properties uncommon in nature, received growing attention from researchers due to their wave manipulation capacities. In particular, engineering their dispersion curves, which relate the wavenumber to the angular frequency, allows for obtaining targeted responses and band-specific vibration attenuation, with applications in a broad range of subjects. While the first studies were mostly focused on interactions between neighbouring unit cells in the periodic substructure, the inclusion of beyond-next-nearest neighbours has broadened the reach of these devices, thanks to their so-called roton-like dispersion relations, which feature local minima and maxima and thus inversion of the sign of the derivative, i.e. the wave envelope velocity. This work extends the previous model by the present authors from one-dimensional monoatomic chains to two-dimensional lattices. Building on the mass conservation principle proposed in the above-mentioned work, this paper applies the previously established mechanical consistency condition to two-dimensional discrete periodic lattices, which is paramount to obtain coherent and comparable models. By applying a mass ratio constraint between the masses of the springs and of the atoms, introduces two dimensionless parameters into the analysis of the bidimensional lattices, α to adjust stiffness distribution and nonlocality level P , based on an homothetic principle for the different configurations. Analytical derivations of dispersion relations as functions of α and P are derived for the five Bravais lattices, and their effects on the dynamical behaviour are discussed. The significance of two-dimensional metamaterials for their versatility and potential for applications as waveguides and elastic wave lenses is undoubted, and by understanding and optimizing the behaviour of two-dimensional metamaterials, new possibilities for advanced materials and devices can be unlocked.

5.1 Introduction

Metamaterials are man-made periodic lattices, which have garnered significant interest for their ability to manipulate waves. This capability has opened up avenues for numerous applications, ranging from vibration filtering to energy harvesting. Two-dimensional metamaterials can be imagined and designed in several ways, depending on engineering needs. Among others, two-dimensional porous metamaterials, such as perforated membranes, are often employed in waveguiding and shielding applications. Their behavior can be tuned by varying the dimensions, shape, and positions of the holes, thus influencing resonance frequency, band gaps, and stop bands ranges. Bar-Sinai et al. [162] study the properties of two-dimensional metamaterials with a nonlinear geometric formulation of elasticity. Nontrivial responses and applications to porous ordered and disordered metamaterials are discussed.

Li et al. [163] focus on the possibility of attaining low frequency wide band gaps, highlighting how geometric tweaking and composite materials allow for significant noise and vibration reduction. The properties of the material geometric designs had in fact already been studied by Mullin [164], who investigated the uniaxial compression behaviour of patterned structures and obtained new configurations of the geometry through critical loads and instability. In the dynamics domain, Langley [165] studied the response of two-dimensional periodic lattices to point harmonic loading, considering both finite and infinite systems, within a damped configuration. A two-dimensional mass-spring lattice is employed to demonstrate analytical calculations agreement with numerical results from finite systems as shells or plates. The author further proposes a lattice made out of elastic bars with periodically varying properties. Another example draws from notions of solid-state physics, such as hexagonal lattices that mimic graphene sheets. Applications include wave focusing, filtering, noise damping and absorption, increased transmission, and energy harvesting. One of the main issues concerning the design of functional metamaterials is however their response informed design, that is, a predictive theoretical procedure that allows for reaching the desired outcomes. Some authors have focused on this purpose, by developing models which are able to plan and foresee the static and dynamic response of wave filtering devices. Among others, Matlack et al. [166] investigate a formal framework to design mechanical metamaterials with desired functionalities, as the target behaviours are often obtained by tweaking material designs and geometries. The goal of their study is to formalise a method that allows to achieve a targeted result by linearly combining elements as one would in an electrical circuit. The metamaterials envisaged are defined as *perturbative*, as the vibration modes of each unit cell differ and can interact with each other, generating couplings that can produce frequency shifts.

Ruzzene et al. [167] evaluated the behaviour of two-dimensional cellular structures, as honeycombs or reticulated frames. The characterization of wave propagation in periodic structures with these geometries is analysed and compared numerically. In the final part of the work an effort is made to identify optimal designs are identified for achieving the desired transmission levels.

In some cases, the lattice properties can be actively tuned and modified through the application of electric or magnetic fields, defining the field of active metamaterials. Nonlinear properties can enhance the static and dynamic performance of metamaterials as well. Employing a two-dimensional continuum model inspired by phase transitions in crystals, Jin et al. [168] studied the transitions in wave shape, velocity and direction in space. By determining the waveform reaction to transition fronts as defects, the authors develop a framework for programmable strongly nonlinear metamaterials.

When thinking of the potential applications for two-dimensional metamaterials, the possibilities are multifold, and waveguides and lenses for elastic waves are especially promising fields. Waveguides are structures designed to confine and guide wave propagation in a desired direction or path. They can be used to create directional band gaps, refraction/deflection, exploiting the interaction between the incident wave and the underlying lattice structure. They allow for focusing and defocusing of elastic waves, similar to their electromagnetic counterparts. Moreover, they can be used to guide vibrational energy to specific points of the lattice. Li et al. [169] studied acoustic confinement and waveguiding in two-dimensional phononic crystals with material defects, i.e., substituting some unit cells with ones with other characteristics. The eigenmodes shifts and the localization of waves at specific frequencies are studied both analytically and numerically, and the modulation of the results through material parameters is shown. Slepnyan et al. [170] provides an insight on the mathematical methods and formulations used in determining the response of waveguides with a substructure and external moving loads.

Lenses can be manufactured to have negative refraction and reflection indices, for instance, with a negative focal distance, which diverts the incident waves. They can also be employed to realize sensors that detect small variations in the mechanical properties of their environment. This was recently demonstrated for elastic waves by Meirbekova et al. [171].

The frequency range of use depends on the envisioned applications and the forcing conditions. Experimental validations of theoretical models, auxetic properties, topological properties, and pro-

grammable metamaterials (active metamaterials) are also important aspects to consider. Bruggi and Corigliano [172] developed an optimization algorithm for two-dimensional auxetic unit cells, thus obtaining an optimal anti-chiral layout with negative Poisson ratio. In prospect, these inverse homogenization method could be applied to waveguide design. Collet and Ruzzene [173] applied a Floquet-Bloch decomposition to damped two-dimensional lattices, in contrast to the undamped systems it is usually employed in. The alternative formulation proposed allows for obtaining the dynamic characteristics of structures with complex damping configurations and design waveguides in presence of damping conditions. Davini et al. [174] propose a two-dimensional honeycomb structure that possesses a synclastic out-of-plane auxetic behaviour that does not match the in-plane one, through appropriate choice of the lattice parameters.

When considering nonlocal connections, evaluating their effect on dispersion surfaces and propagation directions is crucial to be informed on the lattice behaviour under specific loadings. Nonlocal connections in two-dimensional lattice have been investigated to some extent, however there are some aspects still to be uncovered. Zhu et al. [70] apply roton-like connections to a two-dimensional metamaterial for manipulation of acoustic waves. Wang et al. [37] study the wave propagation in two-dimensional nonlocal media, showing that the Fourier analysis can be employed to design the lowest dispersion band for both elastic and sound waves. Moreover the transition behaviour and wave interaction on the boundary between a local and nonlocal lattice, opening a new perspective on waveguiding through long-distance connections.

In this Chapter, with reference to the topic of beyond nearest neighbours connections (BNN) in periodic lattices ([59],[64],[62],[69]) in the field of elastic metamaterial design, and the roton-like behaviour these devices own, the mechanical consistency law presented in [120] is extended to two-dimensional discrete media. As established in Chapter 2, the core importance of mass conservation lies in maintaining the mechanical consistency of the model. Traditional mass-spring models assume that only the masses (atoms) contribute to the inertia of the system, while the springs are considered massless. However, when nonlocal connections are introduced, the mass of the elastic links increases, and if this is not accounted for, it can lead to inaccuracies, as the springs' mass contributes significantly to the system's dynamics. By setting an *a priori* ratio between the overall mass of the atoms and of the springs, it is ensured that the model remains physically sound even when nonlocal interactions are prominent, as the overall available mass to build links on is unchanged. This also enables meaningful comparisons between different metamaterial designs. The conservation law with its tuning parameters α and P is expanded and applied to two-dimensional Bravais lattices through a geometric reasoning based on homothety. Dispersion curves are retrieved for nonlocal two-dimensional lattices and the results are discussed.

5.2 Analysis and Results

In order to examine the impact of BNN connections on the dynamics of discrete periodic systems with a mechanical consistency constraint, simple mass-spring models are employed. The two-dimensional, periodic lattices chosen for this analysis entail only one point-wise mass in each unit cell. The configurations considered are the five Bravais lattices. Bravais lattices are infinite array of points generated through a couple of base vectors, namely the direct lattice vectors, and the five considered correspond to the possible base vector choices. The five different configurations stem from the study of solid state physics, where they represent the possible crystalline arrangement with isomorphic symmetric groups that are not considered equivalent.

Bravais lattices are thus characterised by the orientation and module of the basis vectors in the coordinate space. As in the one-dimensional case, the direct lattice representation is mirrored by a reciprocal lattice representation in the wavenumber domain, where the unit cell corresponds to the first Brillouin zone. In the two-dimensional case a further reduction to the wavenumber range into the

Irreducible Brillouin Zone (IBZ) can be individuated, limited by the so-called high-symmetry points. Both base vectors and high symmetry points for the two-dimensional lattices are illustrated in table 5.1 below.

Type	Base vectors	High symmetry points
Rhombic	$a_1 = a[\sqrt{3}/2, 1/2], a_2 = a[\sqrt{3}/2, -1/2]$	$\Gamma = [0, 0], X = \frac{1}{a}[\pi/2/3, 0], M = \frac{1}{a}[\pi/2, \pi\sqrt{3}/2]$
Oblique	$a_1 = a[1, 0], a_2 = b[\cos\theta, \sin\theta]$	Γ, X, M, Y numerically evaluated
Square	$a_1 = [a, 0], a_2 = [0, a]$	$\Gamma = [0, 0], X = \frac{1}{a}[\pi, 0], M = \frac{1}{a}[\pi, \pi]$
Rectangular	$a_1 = [a, 0], a_2 = [0, b]$	$\Gamma = [0, 0], X = [\pi/a, 0], Y = [0, \pi/b], M = [\pi/a, \pi/b]$
Hexagonal	$a_1 = a[1, 0], a_2 = a[\sqrt{3}/2, 1/2]$	$\Gamma = [0, 0], X = \frac{1}{a}[\pi, \pi/\sqrt{3}], M = \frac{1}{a}[4\pi/3, 0]$

Table 5.1: In the table above the direct lattices and the high symmetry points in the reciprocal lattices for the 5 types of Bravais lattices considered are summarised. For this work, in the oblique case $\theta = \pi/6$.

5.2.1 Mechanical consistency condition

In the previous work by the present authors [120], an investigation of the effects of BNN connections in periodic discrete systems is carried out. A mechanical consistency condition is enforced through a mass-conservation law, that is, keeping the mass of all the links converging in a given bead constant in order to prescribe a fixed ratio between the total masses of respectively springs and atoms to a value $\mu \ll 1$. By doing so, the approximation of mass-spring models, which considers the mass of the springs' negligible to the dynamical behaviour of the system, holds true.

With the further specification of constant material density ρ_s for the springs' constituent material, the above mentioned mechanical consistency condition can be regarded as a volume balance equation for the unit cell:

$$\sum_{j=1}^P \sum_{q=1}^{N(j)} A_j^{(P)} j d_q = V_{const}. \quad (5.1)$$

where P is defined as *level of nonlocality* of the system, d_q is the length of the connection and $N(j)$ is the number of springs for the j^{th} nonlocality level.

This is, however, an equation with a P number of unknowns, namely, the cross-sections of the springs $A_j^{(P)}$, $j \in [1, \dots, P]$, $P \in [1, +\infty[\subseteq \mathbb{N}$. In order to be able to find the areas and to involve one extra degree of tunability, the subsequent hypothesis of mass distribution is plugged into the system, as in the previous cases:

$$A_j^{(P)} = A_1^{(P)} j^{-\alpha}, \quad \alpha \in \mathbb{R}. \quad (5.2)$$

where α is introduced as *stiffness distribution* parameter. This allows for traditional stiffness decrease as the nonlocality level of the considered spring increases, as well as the opposite through negative values of α , which leads to nonlocal links being stiffer than the local ones.

The proposed mass conservation law is easily applied to the unit cell of the 5 Bravais lattices by imposing the volume conservation to the connections to the neighbouring masses in the directions of the lattice base vectors.

In the two-dimensional case, the motion is considered to be out-of-plane and the springs are considered to possess a translational and rotational degree of freedom. It is further assumed that the springs are flexural, and their values are calculated accordingly by plugging the volume-conserving cross-sections derived above into a classical stiffness matrix, the j^{th} spring's stiffness is yielded as

$$\mathbf{K}_{j,q}^{(P)} = \begin{bmatrix} \frac{12EI}{(jd_q)^3} & \frac{6EI}{(jd_q)^2} \\ \frac{6EI}{(jd_q)^3} & \frac{4EI}{(jd_q)} \end{bmatrix} \quad (5.3)$$

later referred as

$$\mathbf{K}_{j,q}^{(P)} = \begin{bmatrix} K_{xx,(j,q)}^{(P)} & K_{x\phi,(j,q)}^{(P)} \\ K_{\phi x,(j,q)}^{(P)} & K_{\phi\phi,(j,q)}^{(P)} \end{bmatrix} \quad (5.4)$$

where for a square cross-section $I = \frac{A_j^{(P)2}}{12}$, or for a circular cross-section with $I_p = \frac{A_j^{(P)2}}{4\pi^2}$. For instance, for a circular section, taking into account the definition of $A_j^{(P)}$ from equations 5.1 and 5.2,

$$I_{p,(j,q)}^{(P)} = \frac{V_{const}^2}{j^{2\alpha} d_q^2 4\pi^2 \sum_{j=1}^P j^{2(1-\alpha)}} \quad (5.5)$$

Subsequently,

$$\begin{aligned} K_{xx,(j,q)}^{(P)} &= \frac{12EV_{const}^2}{d_q^5 j^{3+2\alpha} 4\pi^2 \sum_{j=1}^P j^{2(1-\alpha)}} \\ K_{x\phi,(j,q)}^{(P)} &= \frac{6EV_{const}^2}{d_q^4 j^{2+2\alpha} 4\pi^2 \sum_{j=1}^P j^{2(1-\alpha)}} \\ K_{\phi\phi,(j,q)}^{(P)} &= \frac{4EV_{const}^2}{d_q^3 j^{1+2\alpha} 4\pi^2 \sum_{j=1}^P j^{2(1-\alpha)}} \end{aligned} \quad (5.6)$$

5.2.2 Nonlocality level P through homothety

The nonlocality level can be imposed on a two-dimensional lattice in multiple ways. In this case, a level of nonlocality P is assigned to every *ring*, as they offsets from the unit cell, individuated in masses with positions $r_n = (\pm n_1 a_1, \pm n_2 a_2)$, with $n_1, n_2 \in [0, P] \subseteq \mathbb{N}$, $P \in [1, +\infty[\subseteq \mathbb{N}$. This means that, given the unit mass with coordinates $O = (0, 0)$, a mass will be assigned a j^{th} level of nonlocality when $n_1, n_2 \leq j$. It will thus be possible to each mass to be connected to any other in the area not belonging to the first Brillouin zone of the lattice.

This concept can be formally defined as homothety of the unit cell in the direct lattice, which means that for a nonlocality level $j \in [1, P] \subseteq \mathbb{N}$, $P \in [1, +\infty[\subseteq \mathbb{N}$, the masses connected belong to the j^{th} area with the following properties:

1. Every line is mapped into a parallel line going from the $j^{th} - 1$ to j^{th} nonlocality level. Consequently, angles are unchanged;
2. The ratio between two lines remains constant.

In the same way, it can be formally defined as a *nonlocality window* which expands linearly by scalar multiplication by the nonlocality level $j \in [1, P] \subseteq \mathbb{N}$, $P \in [1, +\infty[\subseteq \mathbb{N}$, whose shape will mirror the unit cell shape given by the basis vectors.

The nonlocality level P for two-dimensional lattices are illustrated in Figure 5.1 below, in the rhombic and square cases.

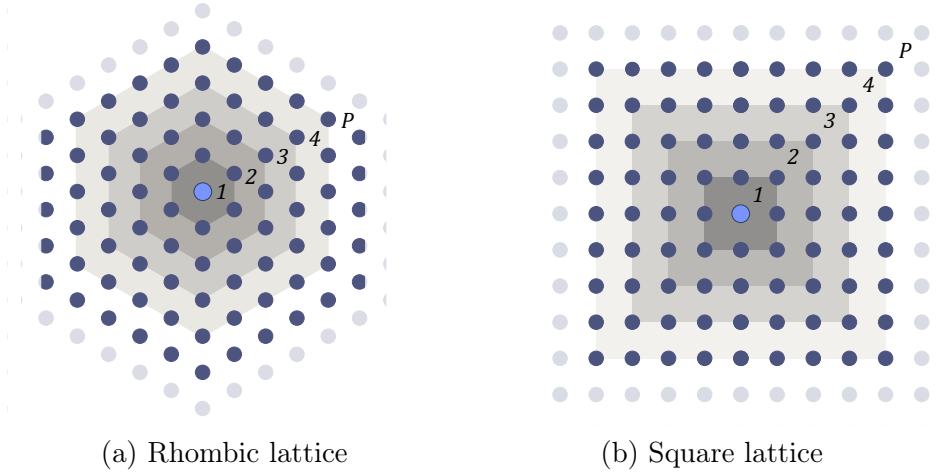


Figure 5.1: *Nonlocality levels in a two-dimensional lattice. The beyond nearest neighbours are considered as a homothetic scaling of the unit cell, whose mass is highlighted in the middle. The example above is illustrated with a rhombic and square lattices, however the same reasoning holds true for every base vectors couple considered.*

Figure 5.2 (a) shows a nonlocal square lattice, which has orthogonal base vectors, while Figure 5.2 (c) shows a nonlocal rhombic lattice, which has an angle $\theta \neq \pi/2$ between the unit lattices of the direct lattice vectors. In the analysis carried out in this section, two kind of lattices are chosen to highlight the key features of BNN connected two-dimensional discrete systems, (a), (c) in Figure 5.2. As illustrated below, these characteristics lead most of the dynamic behaviours of the different Bravais lattices, thus making the behaviour of (b) rectangular, (d) hexagonal and (f) oblique lattices similar in overall behaviour to the two chosen as case studies. However, the considerations in the subsequent paragraphs are valid for these Bravais lattices, and the analysis has been carried out on them as well. The results are gathered in the Appendix to this chapter.

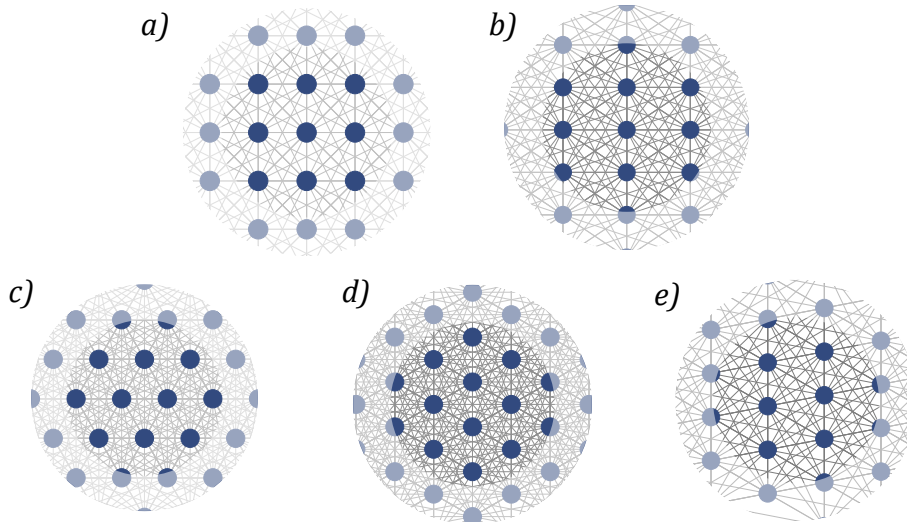


Figure 5.2: *The five two-dimensional Bravais lattices with a nonlocality level $P = 5$ are illustrated above. The nonlocal connections are enforced through homothety, as mentioned above. The letters a), b), c), d), e) correspond to square, rectangular, rhombic, hexagonal and oblique lattices respectively.*

5.2.3 Dynamics

The considered two-dimensional lattice is analysed in a small displacement regime along the x_3 -axis, therefore the dispersion relations are retrieved for out-of-plane vibrations.

$$\sum_{j=1}^P \sum_{q=1}^{N(j)} \mathbf{K}_{j,q}^{(P)} \cdot \mathbf{x}_n = \mathbf{F} \quad (5.7)$$

where P refers to the overall nonlocality level of the lattice, while $N(j)$ to the number of links for every j in that nonlocality window, which will have the same cross-section but not the same length. The atoms in the lattice are considered to have two degrees of freedom (DOFs), with the addition of rotation. The displacements can thus be written as:

$$\mathbf{x}_n = \begin{bmatrix} x_{n,x_3} \\ x_{n,\phi} \end{bmatrix} \quad (5.8)$$

The springs are considered to be flexural and bound to the atoms with a rotational bond. Therefore the equations of motion read:

$$\sum_{j=1}^P \sum_{q=1}^{N(j)} \begin{bmatrix} K_{xx,(j,q)}^{(P)} & K_{x\phi,(j,q)}^{(P)} \\ K_{\phi x,(j,q)}^{(P)} & K_{\phi\phi,(j,q)}^{(P)} \end{bmatrix} \begin{bmatrix} x_{n,x_3} \\ x_{n,\phi} \end{bmatrix} = \begin{bmatrix} F \\ M \end{bmatrix} \quad (5.9)$$

$$\sum_{j=1}^P \sum_{q=1}^{N(j)} \begin{bmatrix} K_{xx,(j,q)}^{(P)} & K_{x\phi,(j,q)}^{(P)} \\ K_{\phi x,(j,q)}^{(P)} & K_{\phi\phi,(j,q)}^{(P)} \end{bmatrix} \begin{bmatrix} x_{n,x_3} \\ x_{n,\phi} \end{bmatrix} = \begin{bmatrix} m\ddot{x} \\ 0 \end{bmatrix} \quad (5.10)$$

By considering the rotational inertia null as with dealing with point masses, $M = 0$ and $x_{n,\phi}$ can be derived from the stiffness values:

$$x_{n,\phi} = - \sum_{j=1}^P \sum_{q=1}^{N(j)} \frac{K_{\phi x,(j,q)}^{(P)}}{K_{\phi\phi,(j,q)}^{(P)}} x_{n,x_3} \quad (5.11)$$

And therefore the equations of motion can be reduced to the following:

$$\sum_{j=1}^P \sum_{q=1}^{N(j)} \left(K_{xx,(j,q)}^{(P)} - K_{x\phi,(j,q)}^{(P)} \frac{K_{\phi x,(j,q)}^{(P)}}{K_{\phi\phi,(j,q)}^{(P)}} \right) x_{n,x_3} = F \quad (5.12)$$

where $F = m\ddot{x}$.

In order to simplify the notation, it is from now on assumed

$$k(j,q)^{(P)} = \left(K_{xx,(j,q)}^{(P)} - K_{x\phi,(j,q)}^{(P)} \frac{K_{\phi x,(j,q)}^{(P)}}{K_{\phi\phi,(j,q)}^{(P)}} \right) \quad (5.13)$$

With this in mind, a solution is assumed as

$$x_n = e^{i(\vec{\kappa} \cdot \vec{r} - \omega t)} \quad (5.14)$$

with $\vec{\kappa}$ being the wavenumber and $\vec{r}$ the position vector, the solution is expressed as a travelling wave.

By imposing periodic boundary conditions in both directions of the lattice basis, the displacements of the neighbouring masses are obtained from the unit cell solution times a phase factor.

$$x_{n+1} = e^{\vec{\kappa} \cdot \vec{r}_n - i\omega t} e^{\vec{\kappa} \cdot \vec{r}_{(n+1)}} \quad (5.15)$$

As in the previous work on the topic of mass conservation and tuneable nonlocal connections [120], the dispersion relations of the proposed models are subject to two parameters: the nonlocality level P and the stiffness distribution parameter α .

The equations of motion, considering a two-dimensional lattice with the above mentioned range of nonlocal connections P , can be written as follows

$$m\ddot{x} = \sum_{j=1}^P \sum_{q=1}^{N(j)} k_{(j,q)}^{(P)} (x_{(j,q)} - x^{(0,0)}), \quad (5.16)$$

with $x^{(0,0)}$ coordinate of the unit cell, and where the stiffness $k_{(j,q)}^{(P)}$ depends on both the stiffness distribution parameter α and the nonlocality level P , and $N(j)$ is number of masses included in the j^{th} level of nonlocality.

5.2.4 Dispersion relation

By using the inner product notation in equation 5.16 and substituting the assumed solutions in equations D.9 and 5.15, the dispersion relation can be expressed as

$$\omega = \sqrt{\frac{1}{m} \left[\sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} (N(j) - e^{i(\vec{\kappa} \cdot \vec{r}_n)}) \right]} \quad (5.17)$$

with r_n position vector of the n^{th} mass of the $N(j)$ masses contained in the j^{th} range of connection, and with $k_{j,q}^{(P)}$ defined in equation 5.13, with length jd_q depending on the distance of the connection. In C supplementary information on the derivation of the dispersion surfaces is presented.

5.3 Results and discussion

The results illustrated in this section refer to the rhombic and square lattices, generated by the a_1, a_2 base vectors graphically shown in Figure 5.3.

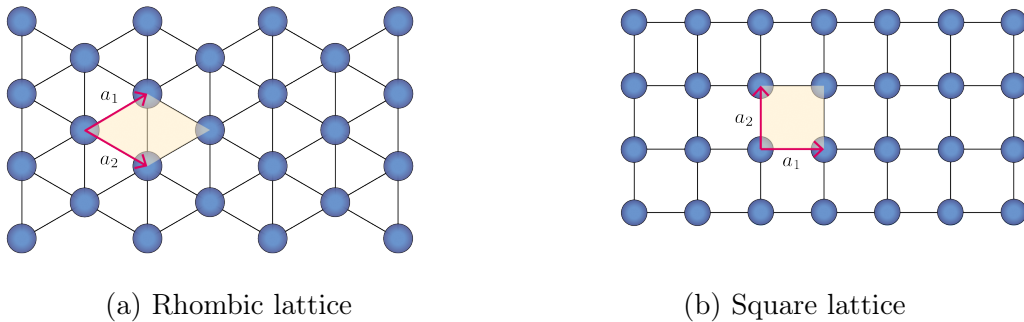


Figure 5.3: A local $P = 1$ rhombic (a) and square (b) lattice.

In Figure 5.4 below, the dispersion relation is shown, as a surface as $\omega = \omega(\kappa_x, \kappa_y)$ is a function of two variables. In 5.4 (a), (b) and (c) the dispersion surfaces for a square Bravais lattice with levels of nonlocality $P = 1, 3, 5$ respectively, and stiffness distribution parameter $\alpha = -5$, are shown, while 5.4 (d), (e) and (f) refer to rhombic lattices with the same α, P parameters.

Figures 5.4 (a) and (d) depict the dispersion surfaces for the local case, where $P = 1$. In this case, the dispersion surface shows an unimodal shape, with the frequency increasing monotonically with the wave number in both directions κ_x, κ_y , which is typical of lattices with only nearest neighbour interactions, but also for nonlocal lattices with high positive α values.

Figure 5.4 (b), (c), (e), and (f) demonstrate the effect of increasing the level of nonlocality, namely $P = 3, 5$ respectively. As P increases, the dispersion surfaces become more complex: the surfaces start to exhibit local minima and maxima, forming valleys and hills. This is a result of the inclusion of beyond-nearest-neighbour interactions (BNN), however it is in this case linked to the value of the stiffness distribution parameter $\alpha = -10$, set to a negative value for the nonlocal links to have sufficient stiffness so that a roton-like dispersion takes place.

As in the monoatomic one-dimensional case, the number of local maxima and minima on the surface is directly proportional to the number of nonlocally connected neighbours, and the depth of the depressions on the surface depends on the value of α .

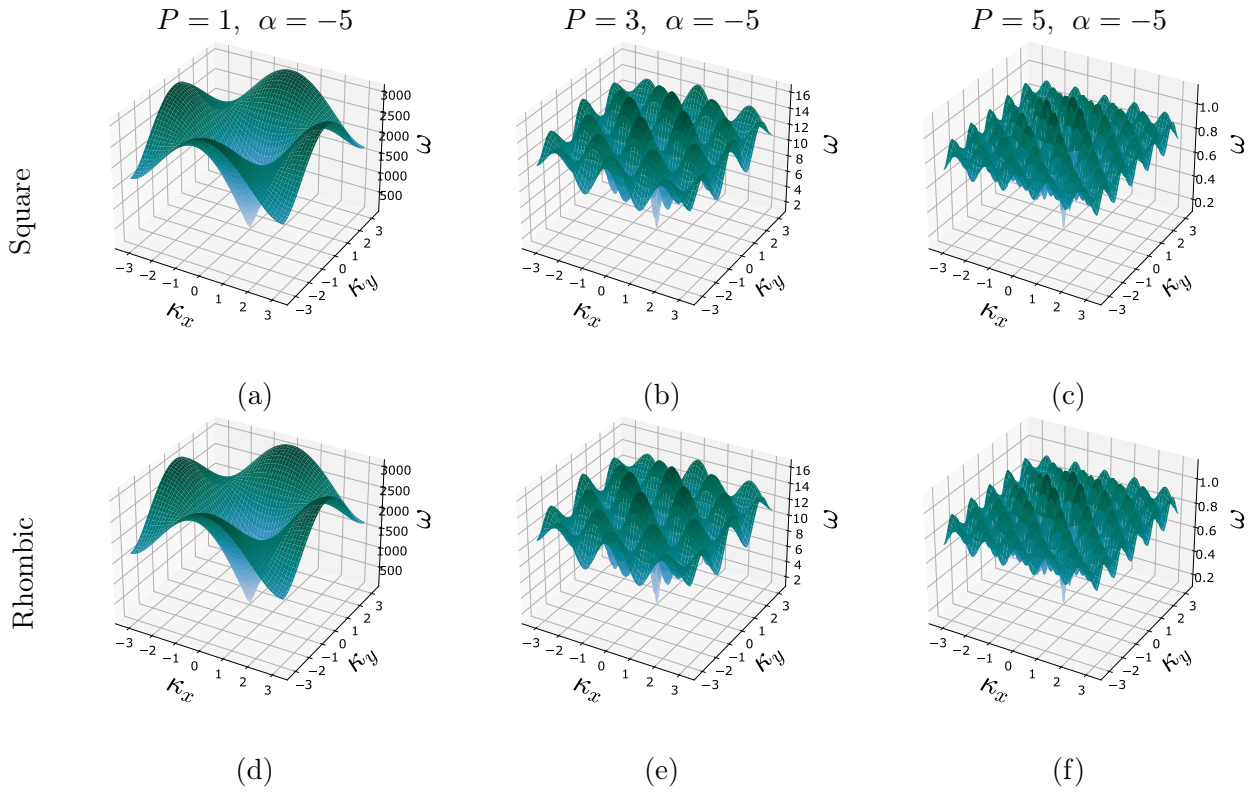


Figure 5.4: Dispersion surfaces for square (a)-(c) and rhombic (d)-(f) lattices, with $P \in [1, 5, 10]$ for $\alpha = -5$. When $P = 1$ the value of α does not impact the frequency range, while in nonlocal lattices the stiffness distribution and thus the dispersion curves can be modified. The figures relate the angular frequency ω [rad/s] to the wavenumbers κ_x, κ_y [rad/m].

The dispersion behaviour can be more clearly observed in the contour plots in Figure 5.5, where the non-monotonic pace of the $\omega = \omega(\kappa_x, \kappa_y)$ frequencies is observed. Figure 5.5 (a), (b) and (c) reports the contour plots of the dispersion relations for a square lattice with $P = 1, 3, 5$ respectively and $\alpha = -10$, while in Figure 5.5 (d), (e), (f) the same parameters are employed to yield the dispersion relations for a rhombic Bravais lattice. Similarly to Figure 5.4, each subfigure illustrates the impact of increasing the level of non-locality P on the dispersion surface. The axes correspond to the wavenumbers κ_x, κ_y in the reciprocal space, while the colourbar indicates the angular frequency value. Figure 5.5 (a) and (d) refer to the local case, where the frequency is seen to increase monotonically in every direction.

On the other hand, Figure 5.5 (b), (c), (e) and (f) refer to the nonlocal case, where local minima and maxima are individuated by colours ranging from dark to light periodically, thus related to the sign inversion of the group velocity.

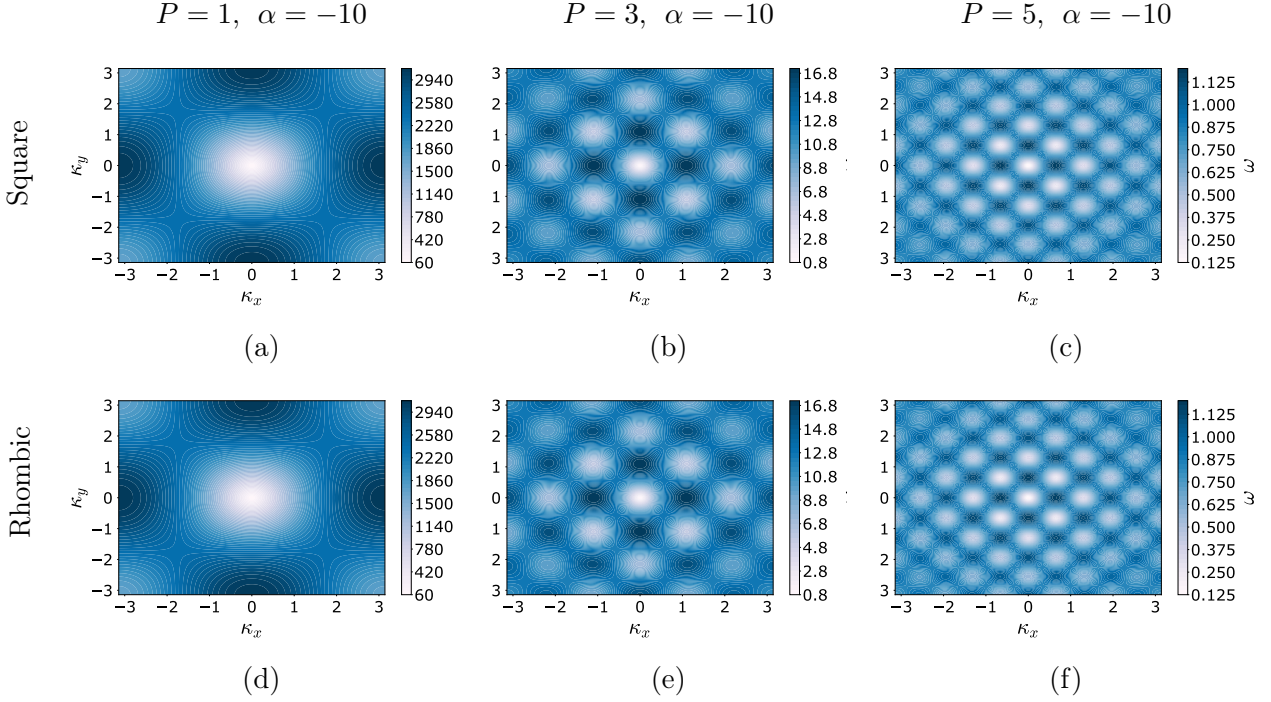


Figure 5.5: Contour plots of the dispersion relations for square (a)-(c) and rhombic (d)-(f) lattices, with $P \in [1, 5, 10]$ for $\alpha = -10$. When $P = 1$ the value of α does not impact the frequency range, while in nonlocal lattices the stiffness distribution and thus the dispersion curves can be modified. The colourbar indicates the frequency value, which is uniformly growing in (a) and (d), while presents multiple rises and falls in the nonlocal models (b), (c), (e) and (f), where the roton-like dispersion is to be found. The figures relate the angular frequency ω [rad/s] to the wavenumbers κ_x, κ_y [rad/m].

5.3.1 Irreducible Brillouin Zones (IBZ)

The Irreducible Brillouin Zone is the first Brillouin zone reduced by all of the symmetries in the lattice, and it is the smallest region in the reciprocal space which contains all of the periodic lattice information. It is possible to visualise the dispersion relation of two-dimensional lattices on a two-dimensional plot by considering a wavevector, namely the reduced wavevector κ_r spanning along the contour of the IBZ, instead of taking into account the full two-dimensional wave vector space κ_x, κ_y . The reduced wavenumber κ_r path along the IBZ contour is obtained by connecting the high-symmetry points Γ, X, M , which differ for the five Bravais lattices and are listed in table 5.1. This path is a one-dimensional representation of the two-dimensional reciprocal space, which enables visualisation of the angular frequency versus wavenumber value along the key directions of propagation in the lattice.

The dispersion relation becomes thus a curve with expression $\omega = \omega(\kappa_r)$. A detailed explanation on lattice symmetries can be found in references [8] and [6].

Figure 5.6 displays the dispersion curves (ω, κ_r) along the IBZ path. This means that the x-axis in each plot does not represent a single direction in reciprocal space but rather a specific path through reciprocal space, connecting the high-symmetry points $\Gamma - X - M$, i.e. the corners of the IBZ.

In Figure 5.6, the dispersion relations along the IBZ contour are shown for the square lattice in (a), (b) and (c), for $P = 1, 3, 5$ respectively, and in (d), (e), (f) for the rhombic lattice. The variations in frequency due to the values of the stiffness distribution parameter α can be noticed. When α assumes

positive values, the dispersion curve resembles the local behaviour even though nonlocal connections are enforced, due to their reduced stiffness.

Figures 5.6 (a) and (d) depict the dispersion curves for the local case, i.e. when $P = 1$. On every path connecting two subsequent high-symmetry points, the curves are monotonic, meaning that the frequency increases with the wave number. This behaviour is consistent with lattices that have only nearest-neighbour interactions.

Figures 5.6 (b), (c), (e) and (f) illustrate the effect of increasing the level of non-locality to $P = 5, 10$ respectively. The increase in the level of non-locality P does not cause the curves along the IBZ path to lose monotonicity, as it happens only when α reaches negative values, from the definition in equation 5.6. If the local links are predominant in the stiffness distribution due to positive α , then the behaviour resembles the local case. On the other hand, when α becomes negative, the stiffness distribution advantages the nonlocal connections and the curves exhibit local minima and maxima, indicating stronger roton-like behaviour.

Local minima in the dispersion curves indicate a negative ratio between the group velocity and the phase velocity of the wave packet, which leads to waves and thus energy propagating backwards in the interested wavenumber ranges. A discussion on the group velocity values in two dimensional lattices is carried out in the subsequent section.

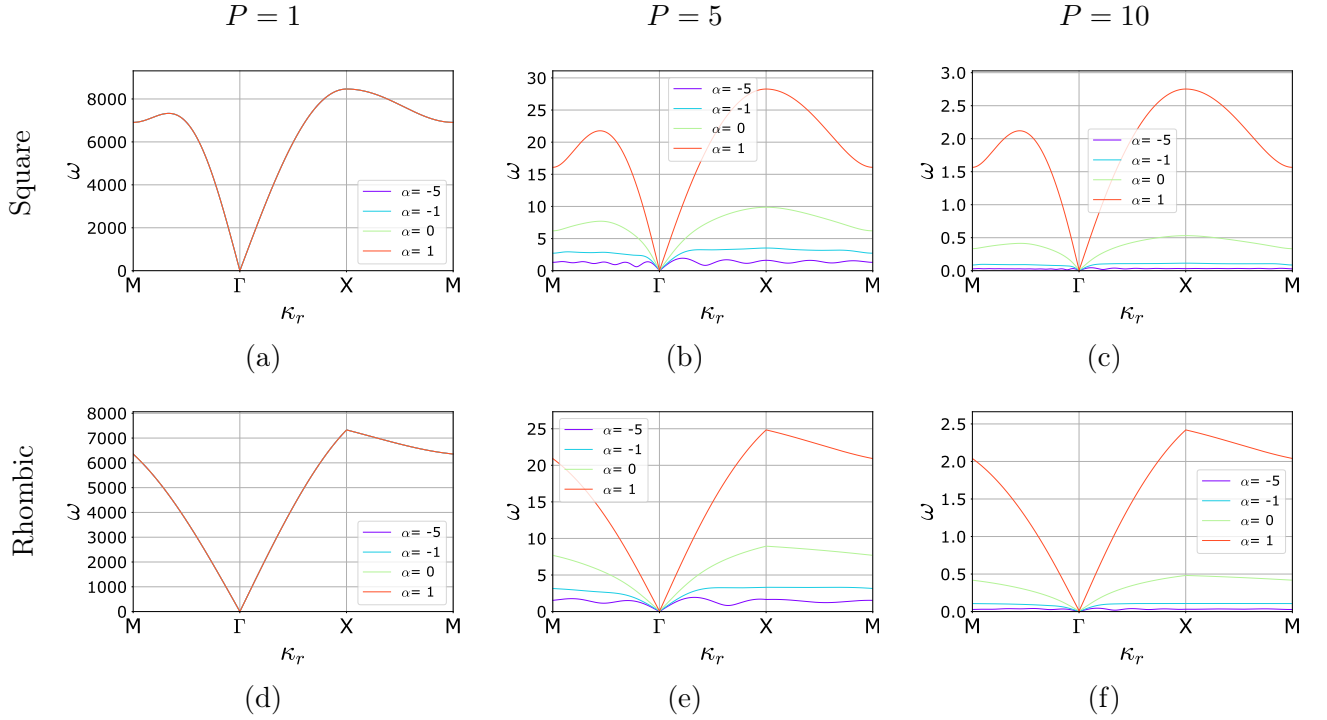


Figure 5.6: Dispersion relations for square (a)-(c) and rhombic (d)-(f) lattices, with $P \in [1, 5, 10]$ for several values of α . When $P = 1$ the value of α does not impact the frequency range, while in nonlocal lattices the stiffness distribution and thus the dispersion curves can be modified. The figures relate the angular frequency ω [rad/s] to the reduced wavenumber κ_r [rad/m].

5.3.2 Wave propagation and group velocity

The direction of propagation of the wave along a lattice is defined by the ratio among the *group velocity* v_{gr} and the *phase velocity* v_{ph} , which define respectively the velocity of the wave envelope and of the wave front. When these two signs do not match, the wave and thus energy propagation happens backwards.

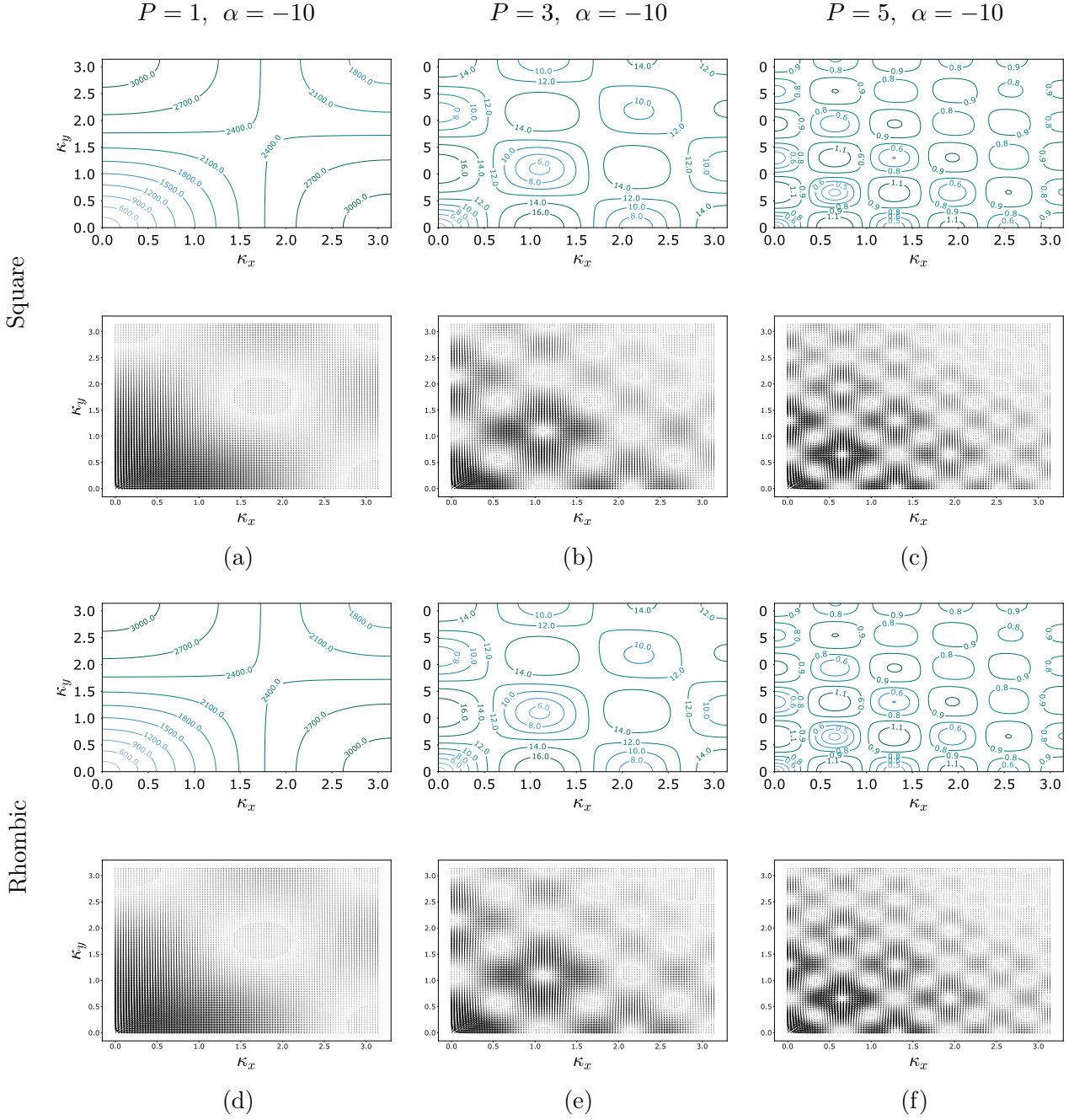


Figure 5.7: Levels of the contour plots of the dispersion surfaces in the positive κ_x, κ_y range (upper figure) and gradient $\nabla\omega$ of the dispersion relations $\omega = \omega(\kappa_x, \kappa_y)$ in the positive κ_x, κ_y range for square (a)-(c) and rhombic (d)-(f) lattices, with $P \in [1, 3, 5]$ for several values of $\alpha = -10$. When $P = 1$ the value of α does not impact the frequency range, while in nonlocal lattices the stiffness distribution and thus the dispersion curves can be modified.

The group and phase velocities are described in one-dimension as

$$v_{gr} = \frac{d\omega}{d\kappa}, \quad v_{ph} = \frac{\omega}{\kappa} \quad (5.18)$$

as the dispersion relation is function of a single variable, $\omega = \omega(\kappa)$. In the two-dimensional case, the dispersion relation is not a curve but a surface, thus a function of two variables, the wavenumbers in

the x, y directions, therefore $\omega = \omega(\kappa_x, \kappa_y)$. Given the positive wavenumber values, as the angular frequency ω has a positive, real value, the wave propagation direction will depend on the sign of the group velocity, i.e. the derivative of the dispersion relation. As the lattice is two-dimensional, this value will vary for every unit vector given by the value of κ_x, κ_y , and thus on the wave propagation direction among the lattice.

The overview of the direction and sign of propagation of the elastic waves is provided by the gradient $\nabla\omega$ of the dispersion surface, which assigns a vector indicating group velocity magnitude, direction and sign to every $[\kappa_x, \kappa_y]$ point in the lattice.

Figure 5.7 provides an overview on the group velocity values based on level contour plots of the dispersion curves (upper figures) and gradient plots (lower figures). The gradient in each point is a vector that indicates the direction and magnitude of the greatest rate of increase (decrease) of the frequency.

Figure 5.7 (a), (b) and (c) show the levels and gradient of the dispersion surface for a rhombic lattice, while Figure 5.7 (d), (e) and (f) refer to a square lattice. Each subfigure represents a different level of non-locality, $P = 1, 5, 10$ respectively.

The group velocity over phase velocity sign can be therefore attained by calculating directional derivatives of the dispersion relation $\omega(\kappa_x, \kappa_y)$ along the directions corresponding to the Γ, X and Γ, M directions along the IBZ, and an array of directions from the points along the discretised X, M path.

The directional derivatives are thus calculated as inner product between the gradient $\nabla\omega$ and the normalised vectors $\mathbf{v}_i$, with N_{dir} number of unit vectors and $i \in N_{dir}$.

$$\frac{\partial\omega}{\partial v_i} = \nabla\omega \cdot \mathbf{v}_i \quad (5.19)$$

From this definition, a study of the sign of the group velocity in two-dimensional lattices can be carried out. In fact, due to the symmetry of the dispersion relation along the main propagation directions, it is possible to analyse the group velocity v_g on an intersection between a plane following one of said directions and the dispersion surface. Without loss of generality, it is possible to study the partial derivative with respect to κ_x along the $\kappa_y = 0$ direction. Reformulated in trigonometric terms considering Euler's formula, it reads

$$\nabla\omega_x(\kappa_x, 0) = \frac{\sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} ((1 - \delta_{1,j})(s_{1,j}) + (s_{2,j}) + (s_{3,j}))}{2m\omega(\kappa_x, 0)} \quad (5.20)$$

where

$$\begin{aligned} s_{3,j} &= 4j \sin(j\kappa_x n_1) \\ s_{2,j} &= 8j \sin(j\kappa_x n_1) \\ s_{1,j} &= \sum_{l=1}^{N_{P-1}} 4(j-l) \sin((j-l)\kappa_x n_1) \end{aligned} \quad (5.21)$$

and $\omega(\kappa_x, 0)$ is the dispersion relation calculated on the $(\kappa_x, 0)$ plane, namely

$$\begin{aligned} \omega &= \left(\frac{1}{m} \left[\sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} (6 \cos(j\kappa_x n_1) - 8 + \right. \right. \\ &\quad \left. \left. + (1 - \delta_{1,j}) \sum_{l=1}^{N_{P-1}} (4 \cos(j\kappa_x n_1) + 4 \cos((j-l)\kappa_x n_1) - 8N_{P-1})) \right] \right)^{1/2} \end{aligned} \quad (5.22)$$

and

are the harmonic components. Without loss of generality, the analysis is restricted to positive wavenumber values $\kappa_x \in [0, \pi/n_1]$. The phase velocity is defined in equation 5.18, and it is thus positive in this range. The sign of the ratio between group and phase velocities is thus dictated by the sign of the latter.

$$sgn\left[\frac{v_{gr}}{v_{ph}}\right] \propto \sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} ((1 - \delta_{1,j})s_{3,j} + s_{2,j} + s_{1,j}) \quad (5.23)$$

Remembering how the stiffness of local and nonlocal links is described in equations 5.6 and 5.13,

$$k_{j,q}^{(P)} = \frac{3EV_{const}^2}{d_q^5 j^{3+2\alpha} 4\pi^2 \sum_{j=1}^P j^{2(1-\alpha)}} \quad (5.24)$$

and the sign proportionality can be expressed as

$$sgn\left[\frac{v_{gr}}{v_{ph}}\right] \equiv sgn\left[\sum_{j=1}^P j^{-2\alpha} \left((1 - \delta_{1,j}) \left(\sum_{l=1}^{N_{P-1}} 4(j-l) \sin((j-l)\kappa_x n_1) \right) + 12j \sin(j\kappa_x n_1) \right) \right] \quad (5.25)$$

where the constant positive values have been neglected. When $P = 1$ and thus $j = 1$, the stiffness distribution parameter α has no effect on the sign of the group velocity, as the sine only has positive values in $[0, \pi]$.

5.3.3 Inequalities

In order to analyse the value of equation 5.25, a dimensionless parameter β is introduced, so that

$$\kappa_x = \frac{\beta\pi}{n_1}, \quad \beta \in [0, 1] \subset \mathbb{R}^+ \quad (5.26)$$

which leads to a dimensionless sign function to be studied in the symmetrical Brillouin zone of positive wavenumbers κ_x , as

$$sgn\left[\frac{v_{gr}}{v_{ph}}\right] \propto \sum_{j=1}^P j^{-2\alpha} \left((1 - \delta_{1,j}) \left(\sum_{l=1}^{N_{P-1}} 4(j-l) \sin((j-l)\beta\pi) \right) + 12j \sin(j\beta\pi) \right) \quad (5.27)$$

The phase difference is governed by the value of β , equal in both terms, while the sign is ruled by the values of j and the sum of the $(j-l)$ terms.

The inner sum over l can be simplified to

$$\sum_{l=1}^{N_{P-1}} 4(j-l) \sin((j-l)\beta\pi) = csc\left(\frac{\beta\pi}{2}\right) (\sin(j\beta\pi) - j(\sin((1-j)\beta\pi) + \sin(j\beta\pi))) \quad (5.28)$$

by manipulating the sine terms through Euler's formula and the finite sum of the geometric series, as summarised in Appendix D. And by bringing the $j = 1$ terms out of the sum, this leads to

$$\text{sgn}\left[\frac{v_{gr}}{v_{ph}}\right] \propto 12\sin(\beta\pi) + \sum_{j=2}^P j^{-2\alpha} \left(\csc\left(\frac{\beta\pi}{2}\right) (\sin(j\beta\pi) + j(\sin((j-1)\beta\pi) - \sin(j\beta\pi)) + 12j \sin(j\beta\pi)) \right) \quad (5.29)$$

The first term is positive in the wavenumber interval considered, therefore for the sign of the ratio to be negative the overall nonlocality level must be $P > 1$. In the sum term, the cosecant is positive for the wavenumber range and the sole out-of-phase term $\forall j$ is $j\sin((j-1)\beta\pi)$.

Therefore, as for $j = 1$ the sign $\text{sgn}\left[\frac{v_{gr}}{v_{ph}}\right]$ is positive, it is clear that nonlocal terms must come into play, and for their stiffness value to weight more than the one of the local links,

$$\alpha < \frac{1}{2} \quad (5.30)$$

is a necessary condition. Thus

$$\forall \alpha \geq \frac{1}{2}, \quad \text{sgn}\left[\frac{v_{gr}}{v_{ph}}\right] \geq 0, \quad \{\forall \beta \in [0, 1] \subset \mathbb{R}^+, \quad \forall P \in [1, +\infty[\subseteq \mathbb{N}\} \quad (5.31)$$

In the context of designing metamaterials that exhibit opposite-sign group and phase velocities, this inequality provides crucial information. It states that, regardless of the nonlocality grade P , two-dimensional lattices with masses connected by elastic springs (which scale according to the stiffness relationship in (5.6), for flexural and rotational springs) can dynamically exhibit roton-like behaviour if and only if the stiffness tuning parameter $\alpha < \frac{1}{2}$.

This work builds upon the mass-conserving model for non-local monoatomic chains introduced by the present authors [120], by exploring the effects of nonlocality in the context of two-dimensional Bravais lattices with the mechanical consistency constraint. The results above display the tuning possibilities provided by the stiffness distribution parameter α and the nonlocality level P .

The presented two-dimensional mass-spring model, while offering some theoretical insights into the impact of establishing a mass-conservation law onto nonlocal discrete lattices, has several limitations that must be considered when interpreting its results and assessing its applicability. Firstly, the model accounts for out-of-plane displacements only, neglecting potential in-plane displacements in two directions. This simplification limits the possibility to capture and exploit a broad range of wave behaviours that might be helpful in a wave manipulating system, where waves can propagate with different polarisations and directions simultaneously. Secondly, the current model is based on a monoatomic unit cell, however multiple dispersion branches and topological modes could be attained by including multiple components in the unit cell of the lattice. An example is in the work of Dal Poggetto et al. [34], where a diatomic lattice composed of two different masses in the unit cell, is considered to study topological bound modes. Furthermore, an experimental validation of the model will involve a three-dimensional prototype that can be approximated as two-dimensional in order for the nonlocal couplings to be taken into account, and not be interlaced with each other, as prospected in literature ([34], [36]). An experimental validation, moreover, would require a numerical validation on finite systems with a discussion on boundary effects due to nonlocality, where generally only the bulk of the lattice can be expected to behave as in the analytical predictions. Further perspectives could include a study on nonlinear effects in the two-dimensional lattice, which is particularly important in the case of acoustical waves and membrane-like behaviour, which could imply large deformations in specific noise attenuation applications. In addition, interface modes and transitions between local and nonlocal lattices, with the parameters α and P introduced above, could provide new insights on the waveguiding and lensing capabilities of the proposed homothetic nonlocal model.

5.4 Conclusions

The mass conservation law previously established is extended to two-dimensional lattice. The *mechanical consistency* criterion ensures that nonlocal connections between elements and the addition of springs proportional to the established nonlocality level P do not interfere with the dynamic and inertial considerations commonly made when working of simplified mass-spring models. Furthermore, the stiffness distribution parameter α , along with the nonlocality level P , provides an additional degree of freedom to tune the dispersion surfaces, thus allowing for the realization of the desired dispersion spectrum and frequency ranges. Moreover, the mass-conservation constraint allows for simple comparisons between configurations of the metamaterial cell, as the dynamic response of multiple lattices with several local and nonlocal configurations can be helpfully designed from the very same amount of material. The presence of local minima and maxima in the dispersion surfaces, which can be emphasized by an appropriate choice of parameters, allows for the creation of areas of backwards propagating energy and energy traps where the group velocity over phase velocity ratio is null, with potential applications to waveguiding and lensing.

The increase in the number of local minima and maxima is tied to the presence of nonlocal couplings, with sufficient stiffness. It is shown that, with the parameters employed in this model, it is necessary for α to have a value $\alpha < \frac{1}{2}$ for the nonlocality effects to take place, as conceptualised in [120].

Compared to other models in literature ([34], [36]), this model enables more connections with neighbouring cells with any level of nonlocality and position. This enables for a larger number of minima and maxima in the dispersion surface, due to sign inversions in the group velocity over phase velocity ratio. The design procedure is compatible with all five of the two-dimensional symmetry groups, i.e. Bravais lattices, and differences between the groups with different angles between base vectors are discussed. Only out-of-plane displacements are enabled, and only one mass unit cells are considered in the lattices, therefore no band gaps arise. A furthering of this work could be thus represented by an expansion of the mass conservation criterion to diatomic two-dimensional lattices, e.g. graphene sheets, and multiple degrees of freedom dynamics. The proposed mass conservation law would allow for a large spectrum of configurations that could be helpfully employed in the design of waveguides, lenses and other devices that combine topological concepts with periodic lattices design, by ensuring that the modelling phase is coherent with the approximations commonly made for local lattices and the availability of material means.

Chapter 6

Conclusive remarks and future perspectives

The hereby presented work was carried out in an attempt to give a physically sound constraint to the modelling of nonlocal models, with dynamical metamaterials in mind.

In Chapter 2, a theoretical framework valid for all of the subsequent chapters has been established. The reasoning was developed on a simple discrete periodic system, i.e. a one-dimensional mass-spring chains. A *mechanical consistency* condition, which is, a physically informed constraint that ensures the validity of the employed discrete mass-springs models, was established. By fixing the ratio between the mass of the springs and of the atoms to a small value, it was ensured that the hypothesis of the springs not participating in the inertial contribution to the dynamics is abided by, even when the number of nonlocal connections increases. Two parameters were introduced, the stiffness distribution parameter α and the nonlocality level P , which rule the mass distribution among the links connecting the atoms, while still maintaining the overall mass value constant for the connections. The governing equations of the periodic discrete system were then analytically formulated through the above-mentioned parameters, and dispersion curves with explicit dependency on α and P were retrieved. Numerical validation through explicit dynamics simulations and 2D FFTs were then attained.

In Chapter 3, the proposed principle was applied to a one-dimensional nonlocal configuration defined as *defected*. The imperfection in the periodic lattice were hypothesised in a shift in the mass distribution either on the beads or the links, with both cases leading to a diatomic unit cell, periodically repeated. As seen in the results section of Chapter 3, this case enabled two branches to appear in the dispersion relation and a bandgap to be created, with presence and width depending on the previously introduced α and P parameters, which govern the analytical formulation. Numerical simulations finally gave an insight of the behaviour of a finite diatomic chain with a further local imperfection.

In Chapter 4, the impact of weak nonlinearities was investigated. The extension of the proposed principle to nonlinear chains was limited to cases where the nonlinearity is small, therefore the analysis was carried out through perturbative methods. By expanding any common nonlinear stress-strain function in series and only considering powers greater than one as perturbations to the linear case, dispersion curves were obtained semi-analytically as a function of the stiffness distribution parameter α and the nonlocality level P . The results were subsequently numerically validated.

In Chapter 5, the mass-conservation approach was finally extended to two-dimensional lattices. Several geometries have been examined, corresponding to the five Bravais lattices that define the main two-dimensional crystallographic groups. The analytical dispersion surfaces with dependency on the α, P parameters were retrieved. Group velocity sign inversion in two-dimensions was discussed.

Overall, the key property of the proposed model is its physical constraint, which allows unusual levels of nonlocal connections while maintaining the validity of a mass-spring model approximation. Once the mass conservation law is established, the transitions between local and nonlocal configura-

tions can be handled in several ways, while keeping the springs' mass negligible compared to one of the atoms. The proposed distribution criterium is based onto the two parameters α and P mentioned above. P refers to the number of nonlocal interactions, i.e. to the unit cells connected beyond the adjacent one, while the stiffness distribution parameter α allows for tuning the mass distribution among the elastic links, advantaging the local or nonlocal ones as its value gears towards positive and negative values respectively. The possibilities of unorthodox situations, where the nonlocal links prevail over the local ones, are highlighted. In fact, for a roton-like dispersion curve to appear in the framework of this model and of the assumed mass-distribution law, nonlocal links must carry a minimum of the total springs' mass, that is found to correspond to a value $\alpha = 0$.

The application of the principle to the imperfect chain holds the same theoretical basis, however a further degree of freedom, i.e. the mass shifts in the atoms or the springs' masses, allows for bandgap creation and tuning through the parameters α, P . Noteworthy, as the roton-like behaviour becomes predominant, bandgaps become discontinuous, therefore ensuring wave propagation in case of undesired manufacturing imperfections. This is due to a roton-like curve both in the acoustical and optical branch. The weakly nonlinear model builds on the same concepts, with a further tunability option given by the amplitude-frequency dependency. Finally, the proposed reasoning is extended to two-dimensional Bravais lattice by an homothetic nonlocality assumption. This means considering a window of nonlocality, as if it were a peridynamic horizon in the continuum case [22], considered as an area of influence directly proportional to the nonlocality level P . All of the unit cells falling into that domain will thus be connected to each other. The roton-like behaviour is found to appear in the dispersion surface and the dispersion curves along the IBZ for negative α values as in the one-dimensional cases. Furthermore, the hypothesis on the springs' behaviour as flexural springs leads to a variation in the stiffness formulation, and thus to the minimum α value to attain negative group velocity to change accordingly.

Regarding future developments of the work carried out in this thesis, multiple paths open up with regard to different aspects that refer to one or more of the models presented. The first limitation that comes to mind is tied to the presence of damping and vibration attenuation in manufactured samples. In fact, complex structures as metamaterial unit cells are built with polymer composites suited to be used in common additive manufacturing and 3D printing. Even considering semi-rigid elastomers and allowing only reduced strains, some damping or hysteretic behaviour is expected, in particular with repeated testing or usage [175]. The importance of considering decaying wave components, i.e. evanescent waves, is discussed in the recent work by Dal Poggetto et al. [176], in which wave propagation in hierarchical viscoelastic plates is investigated. The increase in viscosity generally leads to lower amounts of energy propagating, which can be detrimental or desired based on the expected outcome. For instance, wave attenuation can be exploited to localise and harvest energy. Thorp et al. [177] studied how periodically or aperiodically placing shunted piezoelectric patches along rods can control and attenuate longitudinal wave propagation, whereas Romero García et al. [178] point defects are employed to localise energy and the borders of point defects (cavities) act as mirrors, with evanescent waves generating outside of the cavities.

As thoroughly unfolded in a recent review on topological elastic waveguides [103], the design of periodic systems for wave manipulations can benefit from topological considerations. The work could benefit from an analysis of symmetries (or broken symmetries) in the lattice structures and of how they affect wave propagation, with the emergence of topological modes and their characterization. As defects have been discussed in Part 2, a discussion on interfaces between lattices with different topological invariants and protected modes could give valuable insights, especially in the two-dimensional case where lensing or waveguiding properties could be explored ([170], [179], [166], [180]).

Another theme only briefly mentioned in this Thesis was nonlinearity. Nonlinear metamaterial have displayed interesting features as frequency-amplitude coupling, internal resonance, and the emergence of solitary waves, which are not seen in their linear counterparts, both in local and nonlocal scenarios ([148], [181],[30],[182]). The applications have nonetheless often entailed only weak nonlinearities

([124],[126]), as it was done in this work.

In fact, great amount of caution is necessary when analysing nonlinear vibrations, especially in metamaterials and wave filtering devices, partly due to a lack of predictive tools and the insurgence of undesired phenomena, as chaotic behaviour.

However, applications to strongly nonlinear periodic systems have been observed in granular and impact-based metamaterial designs ([183], [184], [185], [125]).

Nonlinear components have been proven to produce larger vibrations in non-resonance frequencies compared to their linear counterparts, and have been thus employed for energy harvesting purposes [134], [186], [187], Merging topological properties with nonlinearity could broaden the range of capabilities of the nonlocal lattices could reach [188].

A further investigation will thus entail nonlinear properties of strongly nonlinear nonlocal devices, in particular with a focus on nonlinear stress-strain constitutive laws ([189], [190]), the development of ad hoc perturbative tools, and experimental validation. The interest lies in large strains and evanescent waves insurgence attenuation, and in the study of solitons in nonlocal systems.

Furthermore, possible development of the two-dimensional model could involve prestress, leading for instance to a tensegrity design or to a multistable configuration. In literature, prestress has been implemented in devices with wave manipulation purposes already ([191], [192], [193], [194], [195]), and it has proved, among others, to be a valuable tool to induce shifts in the dispersion curves, A possible implementation could follow the footsteps of the model of Miniaci et al. [191], which involves the application of prescribed displacements at the edges of a finite model, thus being able to apply and remove it, achieving a good tunability level. In addition, a study on in-plane vibrations, or both in-plane and out-of-plane modes, could provide information on the interactions of different wave modes in nonlocal systems [27].

Finally, a sensitivity analysis on the boundary effects in discrete finite systems with nonlocal connections is due, as the analyses carried out in this thesis have kept a safety factor with regard to the overall nonlocality level and number of elements constituting the bulk of the periodic lattice ([20], [21]). The transition effects between a strictly nonlocally connected area and one that is only partly nonlocal could be investigated, as well as interface modes, as seen in the work of Wang et al. [36]. The conditions for a rigorous transition from an infinite, i.e. with Bloch-Floquet boundary conditions, to a finite nonlocal lattice should be established.

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Appendices

Appendix A

Analytical derivation of dispersion relations

In the sections below, the analytical and semi-analytical derivations of the dispersion relations discussed in 3 are described in detail.

A.1 Dispersion relation, chains with odd atom masses

Starting from equation 3.8 and employing the Euler formula where $e^{ix} + e^{-ix} = 2\cos(x)$, the system can be rewritten as

$$\begin{aligned}\Omega_1(-\omega^2 + \sum_{j=1}^P 2\frac{k_j^{(P)}}{m_1} - \sum_{j=2}^{P_{even}} 2\frac{k_j^{(P)}}{m_1}(2\cos(j\kappa a)) &= \Omega_2 \sum_{j=1}^{P_{odd}} 2\frac{k_j^{(P)}}{m_1}(2\cos(j\kappa a)) \\ \Omega_2(-\omega^2 + \sum_{j=1}^P 2\frac{k_j^{(P)}}{m_2} - \sum_{j=2}^{P_{even}} 2\frac{k_j^{(P)}}{m_1}(2\cos(j\kappa a)) &= \Omega_1 \sum_{j=1}^{P_{odd}} 2\frac{k_j^{(P)}}{m_2}(2\cos(j\kappa a))\end{aligned}\tag{A.1}$$

For the system to yield nontrivial solutions for Ω_1 and Ω_2 , the following matrix of the coefficients of the system must have null determinant.

$$\begin{bmatrix} -\omega^2 + \sum_{j=1}^P 2\frac{k_j^{(P)}}{m_1} - \sum_{j=2}^{P_{even}} 2\frac{k_j^{(P)}}{m_1}(\cos(j\kappa a)) & -\sum_{j=1}^{P_{odd}} 2\frac{k_j^{(P)}}{m_1}(\cos(j\kappa a)) \\ -\sum_{j=1}^{P_{odd}} 2\frac{k_j^{(P)}}{m_2}(\cos(j\kappa a)) & -\omega^2 + \sum_{j=1}^P 2\frac{k_j^{(P)}}{m_2} - \sum_{j=2}^{P_{even}} 2\frac{k_j^{(P)}}{m_1}(\cos(j\kappa a)) \end{bmatrix}\tag{A.2}$$

The condition on the determinant thus reads

$$\omega^4 - \omega^2\left(\frac{1}{m_1} + \frac{1}{m_2}\right)(-C_1 + C_2) + \frac{1}{m_1 m_2}(C_1^2 + C_2^2 - 4(C_3)^2 - 8C_1 C_2) = 0\tag{A.3}$$

where

$$\begin{aligned}C_1 &= \sum_{j=1}^P 2k_j^{(P)} \\ C_2 &= \sum_{j=2}^{P_{even}} 2k_j^{(P)}(\cos(j\kappa a)) \\ C_3 &= \sum_{j=1}^{P_{odd}} k_j^{(P)}(\cos(j\kappa a))\end{aligned}\tag{A.4}$$

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As the angular frequency ω must have positive values, the quartic equation can be solved for $\bar{\omega} = \omega^2$. The solution for the two dispersion branches $\omega = \omega(\kappa)$ then reads

$$\begin{aligned} \bar{\omega} = & -\left(\frac{1}{m_1} + \frac{1}{m_2}\right)(-C_1 + C_2) \pm \\ & \pm \sqrt{\left(\left(\frac{1}{m_1} + \frac{1}{m_2}\right)(-C_1 + C_2)\right)^2 - \frac{4}{m_1 m_2} (C_1^2 + C_2^2 - 4C_3^2 - 8C_1 C_2)} \end{aligned} \quad (\text{A.5})$$

and substituting the $\bar{\omega} = \omega^2$ values in the equations yields the values of Ω_1 and Ω_2 . Remembering that $m_1 = m + \Delta m$ and $m_2 = m - \Delta m$, equation A.5 becomes

$$\begin{aligned} \bar{\omega} = & -\left(\frac{2m}{m^2 - \Delta m^2}\right)\Delta C \pm \\ & \pm 2\sqrt{\left(\left(\frac{m}{m^2 - \Delta m^2}\right)\Delta C\right)^2 - \frac{1}{m^2 - \Delta m^2} (C_1^2 + C_2^2 - 4C_3^2 - 8C_1 C_2)} \end{aligned} \quad (\text{A.6})$$

where $\Delta C = C_2 - C_1$, and, from the definition of $k_j^{(P)}$ in equation 2.14, the coefficients of the eigenvalue equation can be rewritten as

$$C_1 = \sum_{j=1}^P 2 \frac{EV_{const}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} \quad (\text{A.7})$$

$$C_2 = \sum_{j=2}^{P_{even}} 2 \frac{EV_{const}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} (\cos(j\kappa a)) \quad (\text{A.8})$$

$$C_3 = \sum_{j=1}^{P_{odd}} 2 \frac{EV_{const}}{a^2(j^{1+\alpha})} (\cos(j\kappa a)) \quad (\text{A.9})$$

A.2 Dispersion relation, chains with odd spring masses

Considering the system in equation 3.17, the coefficient matrix follows

$$\begin{bmatrix} -\omega^2 + \frac{1}{m}D_1 - \frac{1}{m}D_2 & -\frac{1}{m}D_4 \\ -\frac{1}{m}D_5 & -\omega^2 + \frac{1}{m}D_1 - \frac{1}{m}D_3 \end{bmatrix}. \quad (\text{A.10})$$

where

$$\begin{aligned} D_1 &= \sum_{j=1}^P (k_{a,j}^{(P)} + k_{b,j}^{(P)}) \\ D_2 &= \sum_{j=2}^{P_{even}} (k_{a,j}^{(P)} e^{i\kappa j a} + k_{b,j}^{(P)} e^{-i\kappa j a}) \\ D_3 &= \sum_{j=2}^{P_{even}} (k_{b,j}^{(P)} e^{i\kappa j a} + k_{a,j}^{(P)} e^{-i\kappa j a}) \\ D_4 &= \sum_{j=1}^{P_{odd}} (k_{a,j}^{(P)} e^{i\kappa j a} + k_{b,j}^{(P)} e^{-i\kappa j a}) \\ D_5 &= \sum_{j=1}^{P_{odd}} (k_{b,j}^{(P)} e^{i\kappa j a} + k_{a,j}^{(P)} e^{-i\kappa j a}). \end{aligned} \quad (\text{A.11})$$

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In this case, the condition on the determinant reads

$$\omega^4 - \frac{\omega^2}{m}(-2D_1 + D_2 + D_3) + \frac{1}{m^2}(D_1^2 + D_2D_3 - D_1D_2 - D_1D_3 - D_4D_5) = 0 \quad (\text{A.12})$$

As the angular frequency ω must have positive values, the quartic equation can be solved for $\bar{\omega} = \omega^2$. The solution for the two dispersion branches $\omega = \omega(\kappa)$ then reads

$$\begin{aligned} \bar{\omega} = & -\frac{1}{m}(-2D_1 + D_2 + D_3) \pm \\ & \pm \sqrt{\left(\frac{1}{m}(-2D_1 + D_2 + D_3)\right)^2 - 4\left(\frac{1}{m^2}(D_1^2 + D_2D_3 - D_1D_2 - D_1D_3 - D_4D_5)\right)} \end{aligned} \quad (\text{A.13})$$

and substituting the $\bar{\omega} = \omega^2$ values in the equations yields the values of Ω_1 and Ω_2 .

Remembering that $k_{a,j}^{(P)} = k_j^{(P)} + \Delta k_j^{(P)}$ and $k_{b,j}^{(P)} = k_j^{(P)} - \Delta k_j^{(P)}$, and that $e^{ij\kappa a} + e^{-ij\kappa a} = 2\cos(j\kappa a)$, $e^{ij\kappa a} - e^{-ij\kappa a} = 2i\sin(j\kappa a)$ the coefficients of the dispersion relation can be reformulated as

$$D1 = \sum_{j=1}^P 2k_j^{(P)} \quad (\text{A.14})$$

$$D2 = \sum_{j=2}^{P_{\text{even}}} 2k_j^{(P)} (\cos(i\kappa a) + i\sin(j\kappa a)) \quad (\text{A.15})$$

$$D3 = \sum_{j=2}^{P_{\text{even}}} 2k_j^{(P)} (\cos(i\kappa a) - i\sin(j\kappa a)) \quad (\text{A.16})$$

$$D4 = \sum_{j=1}^{P_{\text{odd}}} 2k_j^{(P)} (\cos(i\kappa a) + i\sin(j\kappa a)) \quad (\text{A.17})$$

$$D5 = \sum_{j=1}^{P_{\text{odd}}} 2k_j^{(P)} (\cos(i\kappa a) - i\sin(j\kappa a)) \quad (\text{A.18})$$

and from equations ?? and ??,

$$D1 = \sum_{j=1}^P 2 \frac{EV_{\text{const}}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} \quad (\text{A.19})$$

$$D2 = \sum_{j=2}^{P_{\text{even}}} 2 \frac{EV_{\text{const}}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} (\cos(i\kappa a) + i\sin(j\kappa a)) \quad (\text{A.20})$$

$$D3 = \sum_{j=2}^{P_{\text{even}}} 2 \frac{EV_{\text{const}}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} (\cos(i\kappa a) - i\sin(j\kappa a)) \quad (\text{A.21})$$

$$D4 = \sum_{j=1}^{P_{\text{odd}}} 2 \frac{EV_{\text{const}}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} (\cos(i\kappa a) + i\sin(j\kappa a)) \quad (\text{A.22})$$

$$D5 = \sum_{j=1}^{P_{\text{odd}}} 2 \frac{EV_{\text{const}}}{a^2(j^{1+\alpha}) \sum_{j=1}^P j^{1-\alpha}} (\cos(i\kappa a) - i\sin(j\kappa a)) \quad (\text{A.23})$$

in which the dependency on the stiffness distribution parameter α is explicit.

A.3 Solution to the generalization to a N masses unit cell, BNN couplings

A periodic system can be described by its unit cell, whose displacement times a phase factor yields the displacement at another point of the system. This stems from the Bloch-Floquet periodic boundary conditions for periodic lattices, as described for mass-spring systems in the work of Brillouin [8]. For a single mass unit cell the following equation gives the displacement at the n^{th} position by adding a phase factor to the known displacement of the unit cell $x_n(t)$:

$$x_n(t) = e^{i\kappa(m-n)a} x_m(t) \quad (\text{A.24})$$

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where κ is the wavenumber, and a the unit cell spacing.

A system which contains N masses in its unit cell is described by the following system, which relates the masses to their counterparts in the preceding and following unit cells

$$x_n(t) = e^{i\kappa na - i\omega t} \times \begin{cases} a_{k1} & n = 2s, \quad s \in \mathbb{Z} \\ a_{k2} & n = 2s + 1, \quad s \in \mathbb{Z} \\ \vdots \\ a_{kN} & n = 2s + (N - 1), \quad s \in \mathbb{Z}, \end{cases} \quad (\text{A.25})$$

for N number of masses and a_{ki} , $i \in N$ wave amplitudes.

The phase factor is therefore defined over the length of the unit cell $L = Na$, as

$$e^{ikNa}$$

The Newton equations of motion of the system can be written in the compact form that follows,

$$\mathbf{M} \cdot \ddot{\mathbf{x}} = \mathbf{K} \cdot \mathbf{x},$$

where $\mathbf{M}$ is the diagonal $N \times N$ mass matrix and $\mathbf{K}$ the $N \times N$ stiffness matrix. It thence contains equations of this kind, for i masses, with reference to the n_{th} unit cell:

$$\begin{cases} m_{a_{k1}} \ddot{x}_n = k_1(\ddot{x}_{n+1} - \ddot{x}_n) + k_i(\ddot{x}_{n-1} - \ddot{x}_n) \\ \vdots \\ m_{a_{kN}} \ddot{x}_{n+N-1} = k_i(\ddot{x}_{n+1} - \ddot{x}_n) + k_{N-1}(\ddot{x}_{n-1} - \ddot{x}_n) \end{cases} \quad (\text{A.26})$$

Substituting the solution A.24 in the system, the system follows

$$\begin{cases} -m_{a_{k1}} \omega^2 a_{k1} = k_1(a_{k2} - a_{k1}) + k_p(a_{kj} e^{-ikNa} - a_{k1}) \\ \vdots \\ -m_{a_{kN}} \omega^2 a_{kN} = k_N(a_{k1} e^{ikNa} - a_{kN}) + k_{N-1}(a_{kN-1} - a_{kN}) \end{cases} \quad (\text{A.27})$$

For a local system the stiffness matrix is diagonal, while as the number of beyond nearest neighbour pairings increases, the $\mathbf{K}$ matrix becomes more spread out till no zero elements are left, with Floquet-Bloch operators on connections which refer to elements in previous and following unit cells.

$$\begin{bmatrix} \sum k_p & -k_1 - \sum k_j e^{-ikNa} & \dots & -k_n - \sum k_r e^{-ikNa} \\ -k_1 - \sum k_l e^{ikNa} & \sum k_p & \dots & -k_t - \sum k_s e^{-ikNa} \\ \vdots & \vdots & \ddots & \vdots \\ -k_n - \sum k_j e^{ikNa} & -k_2 - \sum k_m e^{ikNa} & \dots & \sum k_p \end{bmatrix} \quad (\text{A.28})$$

The eigenproblem then reads

$$\omega^2 = \mathbf{K} \mathbf{M}^{-1} \quad (\text{A.29})$$

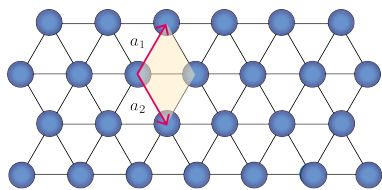
Solving the eigenvalue problem yields the eigenfrequencies for each wavenumber, and thus dispersion relation of the unit cell, with N branches corresponding to N degrees of freedom.

Appendix B

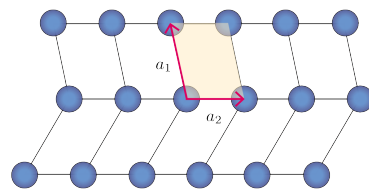
Supplementary results for Bravais lattices

In the subsections below, the results for the Bravais lattices not described above are illustrated.

B.0.1 Hexagonal and oblique lattices



(a) Hexagonal lattice



(b) Oblique lattice

Figure B.1: A local $P = 1$ Hexagonal (a) and oblique (b) lattice.

Appendix B. Supplementary results for Bravais lattices

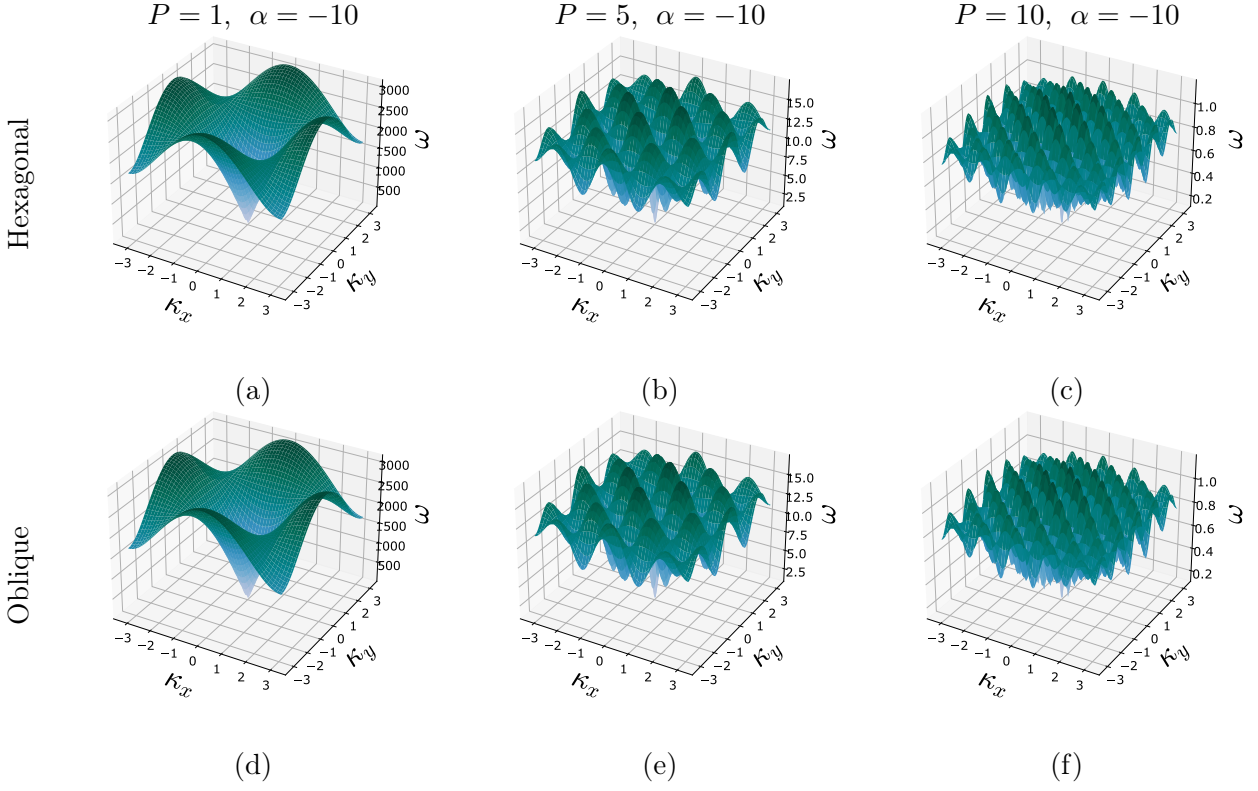


Figure B.2: Dispersion surfaces for hexagonal (a)-(c) and oblique (d)-(f) lattices, with $P \in [1, 5, 10]$ for $\alpha = -10$. When $P = 1$ the value of α does not impact the frequency range, while in nonlocal lattices the stiffness distribution and thus the dispersion curves can be modified.

Appendix B. Supplementary results for Bravais lattices

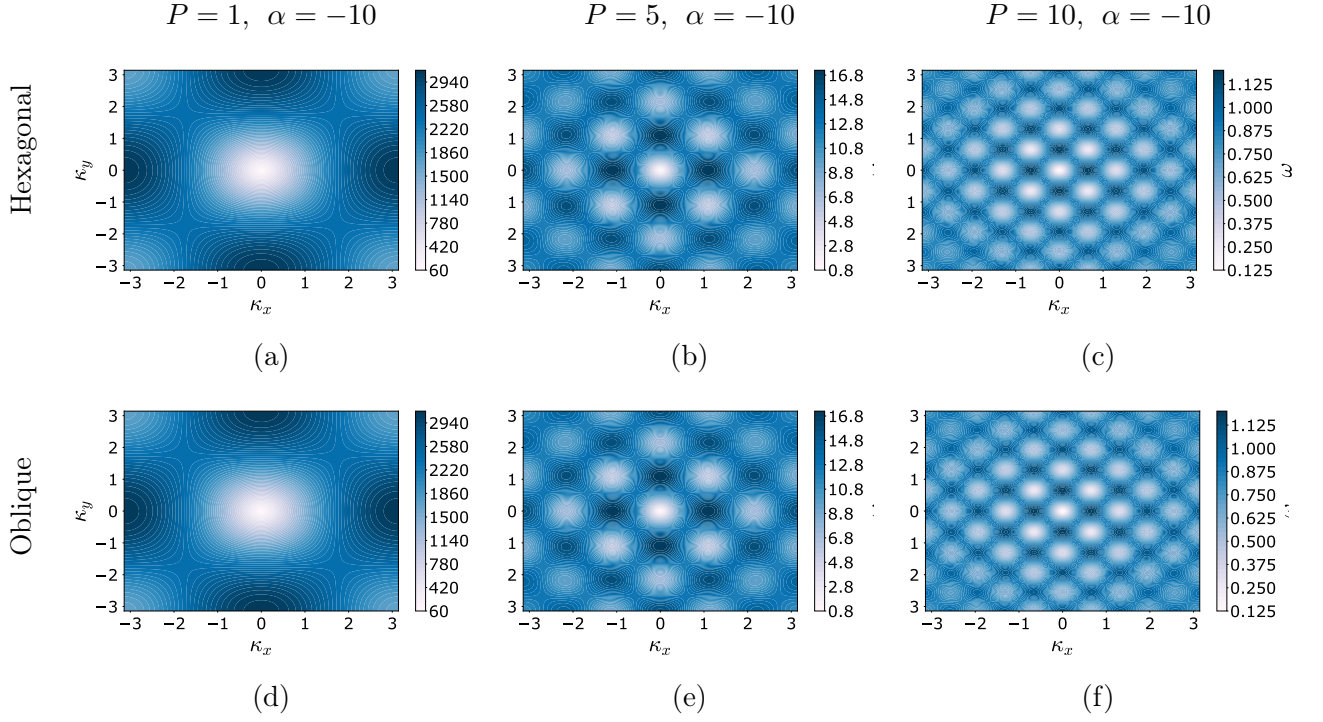


Figure B.3: Contour plots of the dispersion relations for hexagonal and oblique lattices, with $P \in [1, 5, 10]$ for $\alpha = -10$. When $P = 1$ the value of α does not impact the frequency range, while in nonlocal lattices the stiffness distribution and thus the dispersion curves can be modified.

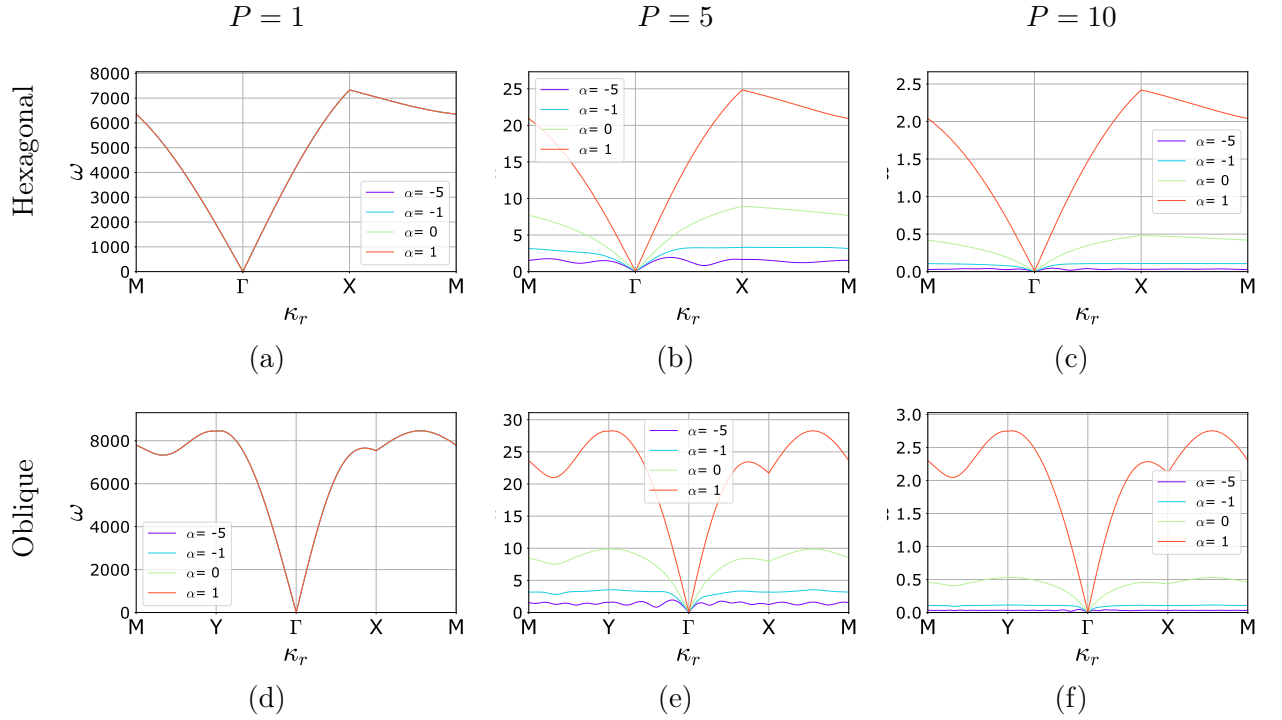
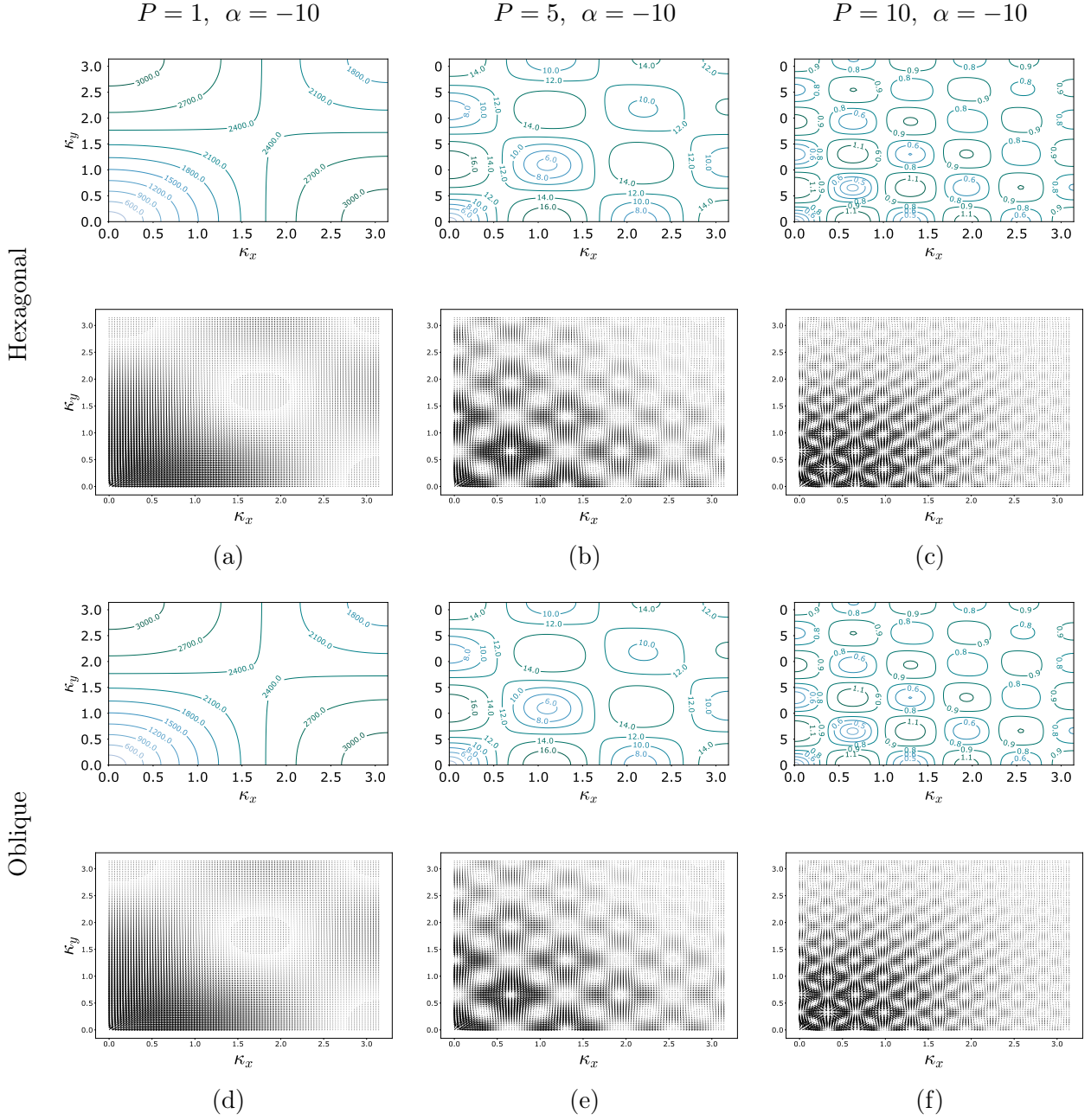


Figure B.4: Dispersion relations for hexagonal (a)-(c) and oblique (d)-(f) lattices, with $P \in [1, 5, 10]$ for several values of α . When $P = 1$ the value of α does not impact the frequency range, while in nonlocal lattices the stiffness distribution and thus the dispersion curves can be modified.

Appendix B. Supplementary results for Bravais lattices



B.0.2 Rectangular lattices

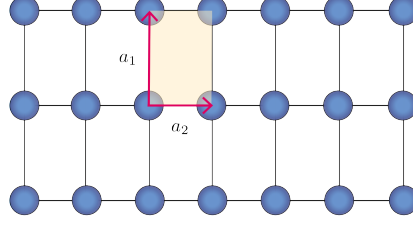


Figure B.6: A local $P = 1$ rectangular lattice.

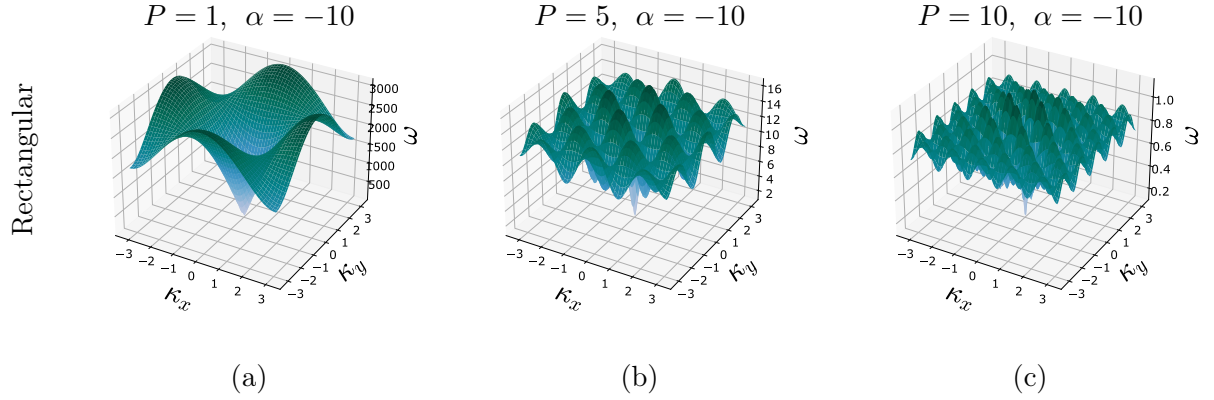


Figure B.7: Dispersion surfaces for rectangular lattices, with $P \in [1, 5, 10]$ for $\alpha = -10$. When $P = 1$ the value of α does not impact the frequency range, while in nonlocal lattices the stiffness distribution and thus the dispersion curves can be modified.

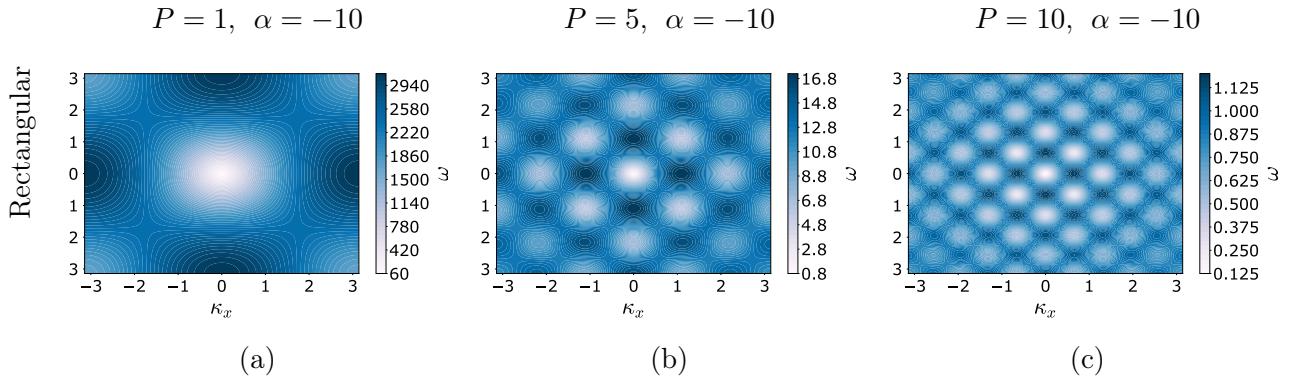


Figure B.8: Contour plots of the dispersion relations for rhombic and square lattices, with $P \in [1, 5, 10]$ for $\alpha = -10$. When $P = 1$ the value of α does not impact the frequency range, while in nonlocal lattices the stiffness distribution and thus the dispersion curves can be modified.

Appendix B. Supplementary results for Bravais lattices

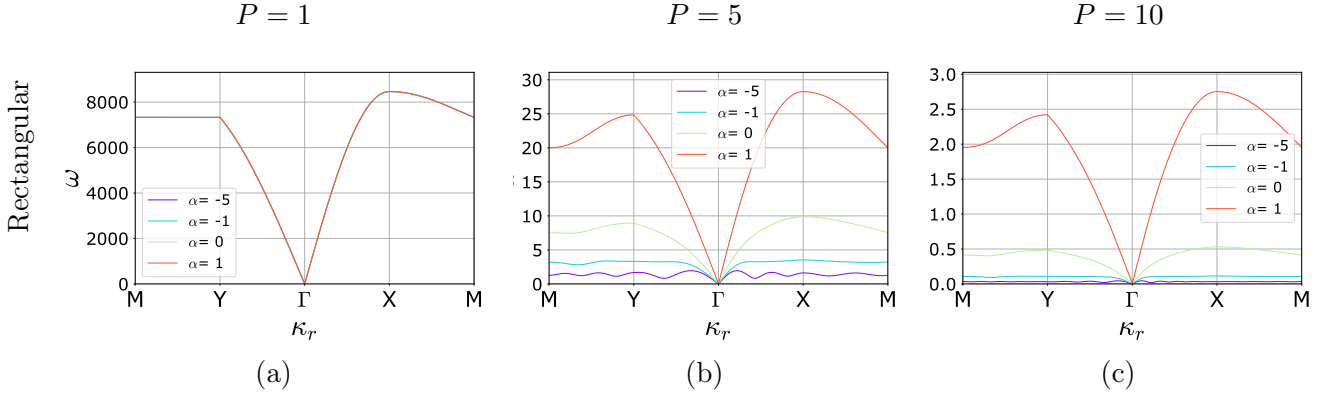


Figure B.9: Dispersion relations for rectangular lattices, with $P \in [1, 5, 10]$ for several values of α . When $P = 1$ the value of α does not impact the frequency range, while in nonlocal lattices the stiffness distribution and thus the dispersion curves can be modified.

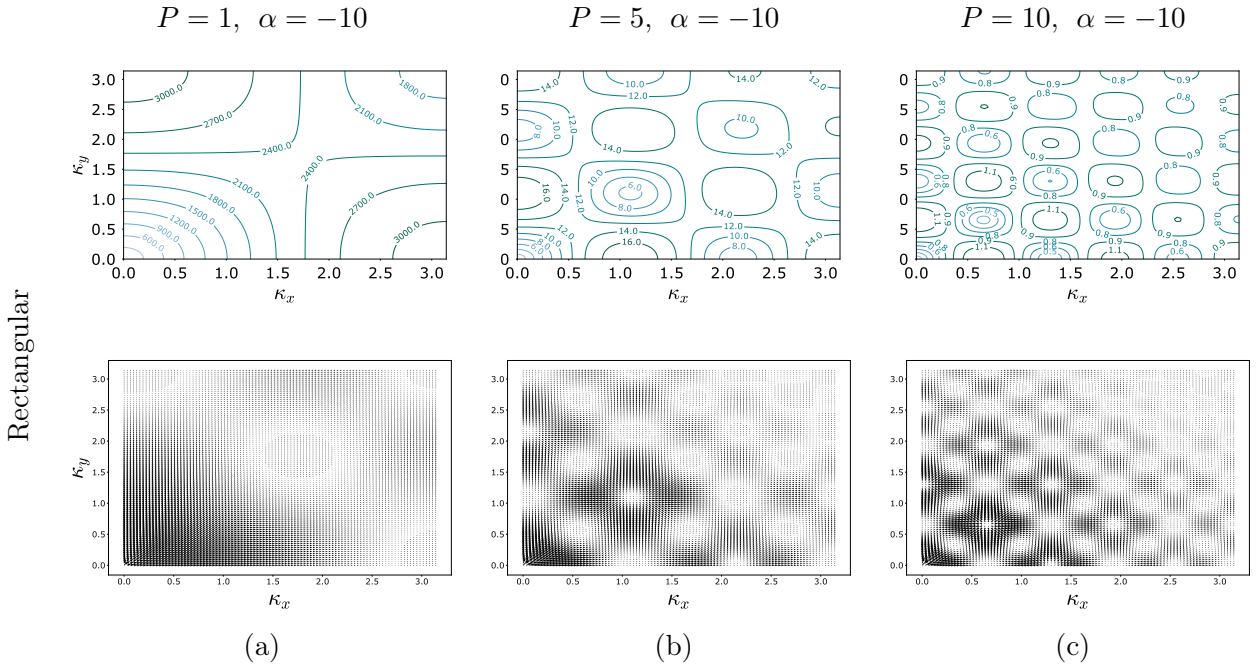


Figure B.10: Levels of the contour plots of the dispersion surfaces in the positive κ_x, κ_y range (upper figure) and gradient $\nabla\omega$ of the dispersion relations $\omega = \omega(\kappa_x, \kappa_y)$ in the positive κ_x, κ_y range for rectangular lattices, with $P \in [1, 3, 5]$ for several values of $\alpha = -10$. When $P = 1$ the value of α does not impact the frequency range, while in nonlocal lattices the stiffness distribution and thus the dispersion curves can be modified.

Appendix C

Supplementary mathematics

C.0.1 Dispersion relation

The equations of motion of the unit cell of the nonlocal Bravais lattices can be formulated as:

$$\begin{aligned}
m\ddot{x}^{(0,0)} = & \sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} (x^{(j,j)} + x^{(-j,j)} + x^{(j,-j)} + x^{(-j,-j)} - 4x^{(0,0)}) \\
& + \sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} (x^{(j,0)} + x^{(-j,0)} + x^{(0,j)} + x^{(0,-j)} - 4x^{(0,0)}) \\
& + \sum_{j=1}^P \sum_{q=1}^{N(j)} (1 - \delta_{1,j}) k_{j,q}^{(P)} \left[\left(\sum_{l=1}^{N_{P-1}} x^{(j,l-j)} + x^{(-j,l-j)} + x^{(l-j,j)} + x^{(l-j,-j)} \right. \right. \\
& \left. \left. + x^{(j,j-l)} + x^{(-j,j-l)} + x^{(j-l,j)} + x^{(j-l,-j)} \right) - 8N_{P-1}x^{(0,0)} \right]
\end{aligned} \tag{C.1}$$

where the Kronecker $\delta_{1,j}$ is defined on row one as

$$\begin{aligned}
\delta_{1,j} &= 0 \quad \text{if } j \neq 1 \\
\delta_{1,j} &= 1 \quad \text{if } j = 1
\end{aligned} \tag{C.2}$$

From D.9 and 5.15, one can plug the traveling wave solution into the equations of motion as

$$\begin{aligned}
-\omega^2 m = & \sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} (e_{1,j} - 4) + \sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} (e_{2,j} - 4) + \\
& + \sum_{j=1}^P \sum_{q=1}^{N(j)} (1 - \delta_{1,j}) k_{j,q}^{(P)} (e_{3,j} + e_{4,j} - 8N_{P-1})
\end{aligned} \tag{C.3}$$

where

Appendix C. Supplementary mathematics

$$\begin{aligned}
e_{1,j} &= e^{i(j\kappa_x n_1 + j\kappa_y n_2)} + e^{i(-j\kappa_x n_1 + j\kappa_y n_2)} + \\
&\quad + e^{i(j\kappa_x n_1 - j\kappa_y n_2)} + e^{i(-j\kappa_x n_1 - j\kappa_y n_2)} \\
e_{2,j} &= e^{i(j\kappa_x n_1)} + e^{i(-j\kappa_x n_1)} + e^{i(j\kappa_y n_2)} + e^{i(-j\kappa_y n_2)} \\
e_{3,j} &= \sum_{l=1}^{P-1} e^{i(j\kappa_x n_1 + (l-j)\kappa_y n_2)} + e^{i(-j\kappa_x n_1 + (l-j)\kappa_y n_2)} + \\
&\quad + e^{i((l-j)\kappa_x n_1 + j\kappa_y n_2)} + e^{i((l-j)\kappa_x n_1 - j\kappa_y n_2)} \\
e_{4,j} &= \sum_{l=1}^{P-1} e^{i(j\kappa_x n_1 + (j-l)\kappa_y n_2)} + e^{i(-j\kappa_x n_1 + (j-l)\kappa_y n_2)} + \\
&\quad + e^{i((j-l)\kappa_x n_1 + j\kappa_y n_2)} + e^{i((j-l)\kappa_x n_1 - j\kappa_y n_2)}
\end{aligned} \tag{C.4}$$

having considered that

$$\vec{\kappa} \cdot \vec{r}_n = (\kappa \cdot a_1)n_1 + (\kappa \cdot a_2)n_2 = \kappa_x n_1 + \kappa_y n_2. \tag{C.5}$$

The dispersion relation can thus be written as

$$\omega = \sqrt{\frac{1}{m} \left[\sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} (8 - e_{1,j} - e_{2,j}) + \sum_{j=1}^P \sum_{q=1}^{N(j)} (1 - \delta_{1,j}) k_{j,q}^{(P)} (8N_{P-1} - e_{3,j} - e_{4,j}) \right]} \tag{C.6}$$

or, by using the inner product notation, it can be summarised as

$$\omega = \sqrt{\frac{1}{m} \left[\sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} (N(j) - e^{i(\vec{\kappa} \cdot \vec{r}_n)}) \right]} \tag{C.7}$$

with r_n position vector of the n^{th} mass of the $N(j)$ masses contained in the j^{th} range of connection, and with $k_{j,q}^{(P)}$ defined in equation 5.13, with length jd_q depending on the distance of the connection.

C.0.2 Gradient

The components of the gradient read:

$$\begin{aligned}
\nabla \omega_x &= \frac{\sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} \left((1 - \delta_{1,j}) \left(\frac{\partial e_{3,j}}{\partial \kappa_x} + \frac{\partial e_{4,j}}{\partial \kappa_x} \right) + \frac{\partial e_{2,j}}{\partial \kappa_x} + \frac{\partial e_{1,j}}{\partial \kappa_x} \right)}{2\sqrt{m \sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} (8 - e_{1,j} - e_{2,j} + (1 - \delta_{1,j})(8N_{P-1} - e_{3,j} - e_{4,j}))}} \\
\nabla \omega_y &= \frac{\sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} \left((1 - \delta_{1,j}) \left(\frac{\partial e_{3,j}}{\partial \kappa_y} + \frac{\partial e_{4,j}}{\partial \kappa_y} \right) + \left(\frac{\partial e_{2,j}}{\partial \kappa_y} + \frac{\partial e_{1,j}}{\partial \kappa_y} \right) \right)}{2\sqrt{m \sum_{j=1}^P \sum_{q=1}^{N(j)} k_{j,q}^{(P)} (8 - e_{1,j} - e_{2,j} + (1 - \delta_{1,j})(8N_{P-1} - e_{3,j} - e_{4,j}))}},
\end{aligned} \tag{C.8}$$

where

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$$\begin{aligned}
\frac{\partial e_{1,j}}{\partial \kappa_x} &= ij(e^{i(j\kappa_x n_1 + j\kappa_y n_2)} + e^{i(j\kappa_x n_1 - j\kappa_y n_2)} + \\
&\quad - e^{i(-j\kappa_x n_1 + j\kappa_y n_2)} - e^{i(-j\kappa_x n_1 - j\kappa_y n_2)}) \\
\frac{\partial e_{2,j}}{\partial \kappa_x} &= ij(e^{ij\kappa_x n_1} - e^{-ij\kappa_x n_1}) \\
\frac{\partial e_{3,j}}{\partial \kappa_x} &= \sum_{l=1}^{N_P-1} i(l-j)(e^{i((l-j)\kappa_x n_1 - j\kappa_y n_2)} + e^{i((l-j)\kappa_x n_1 + j\kappa_y n_2)} + \\
&\quad - e^{i((j-l)\kappa_x n_1 - j\kappa_y n_2)} - e^{i((j-l)\kappa_x n_1 + j\kappa_y n_2)}) \\
\frac{\partial e_{4,j}}{\partial \kappa_x} &= \sum_{l=1}^{N_P-1} ij(e^{i(j\kappa_x n_1 + (l-j)\kappa_y n_2)} - e^{i(-j\kappa_x n_1 + (l-j)\kappa_y n_2)} + \\
&\quad + e^{i(j\kappa_x n_1 + (j-l)\kappa_y n_2)} - e^{i(-j\kappa_x n_1 + (j-l)\kappa_y n_2)}) \\
\frac{\partial e_{1,j}}{\partial \kappa_y} &= ij(e^{i(j\kappa_x n_1 + j\kappa_y n_2)} - e^{i(j\kappa_x n_1 - j\kappa_y n_2)} + \\
&\quad + e^{i(-j\kappa_x n_1 + j\kappa_y n_2)} - e^{i(-j\kappa_x n_1 - j\kappa_y n_2)}) \\
\frac{\partial e_{2,j}}{\partial \kappa_y} &= ij(e^{ij\kappa_y n_2} - e^{-ij\kappa_y n_2}) \\
\frac{\partial e_{3,j}}{\partial \kappa_y} &= \sum_{l=1}^{N_P-1} ij(-e^{i((l-j)\kappa_x n_1 - j\kappa_y n_2)} + e^{i((l-j)\kappa_x n_1 + j\kappa_y n_2)} + \\
&\quad - e^{i((j-l)\kappa_x n_1 - j\kappa_y n_2)} + e^{i((j-l)\kappa_x n_1 + j\kappa_y n_2)}) \\
\frac{\partial e_{4,j}}{\partial \kappa_y} &= \sum_{l=1}^{N_P-1} (l-j)(e^{i(j\kappa_x n_1 + (l-j)\kappa_y n_2)} + e^{i(-j\kappa_x n_1 + (l-j)\kappa_y n_2)} + \\
&\quad - e^{i(j\kappa_x n_1 + (j-l)\kappa_y n_2)} - e^{i(-j\kappa_x n_1 + (j-l)\kappa_y n_2)})
\end{aligned} \tag{C.9}$$

Appendix D

Simplification of the group velocity expression

In order to analyse the sign of equation 5.29, it was convenient to reduce the following sum to its overall value,

$$S = \sum_{l=1}^{N_{P-1}} (j-l) \sin((j-l)\beta\pi). \quad (\text{D.1})$$

The sum can be reduced to a finite geometric series by rewriting the summation indeces as

$$\begin{aligned} k &= j - l \\ l = 1 &\implies k = j - 1 \\ l = j - 1 &\implies k = 1 \end{aligned} \quad (\text{D.2})$$

Therefore, equation D.1 can be rewritten as

$$\sum_{k=1}^{j-1} k \sin(k\beta\pi), \quad (\text{D.3})$$

and knowing that $e^{ix} = \cos x + i \sin x$, the sine term above can be considered as the imaginary part of an exponential function. To simplify calculation, the real part is thus added to sum in equation to yield the exponential form.

$$\sum_{k=1}^{j-1} k e^{k\beta\pi}. \quad (\text{D.4})$$

It is well known that the result of a finite geometric sum can be calculated as

$$\sum_{k=1}^N a^k = \frac{a(a^N - 1)}{a - 1}, \quad (\text{D.5})$$

however, considering $a = e^{i\beta\pi}$, the sum in equation D.4 has the form

$$S = \sum_{k=1}^N k a^k = a + 2a^2 + \dots + (N-1)a^{N-1} + Na^N. \quad (\text{D.6})$$

By writing

Appendix D. Simplification of the group velocity expression

$$a \cdot S = a^2 + 2a^3 + \dots + (N-1)a^N + Na^{N+1} \quad (\text{D.7})$$

one can write $(a-1)S$ as

$$(a-1)S = Na^{N+1} - \frac{a(a^N - 1)}{a-1}, \quad (\text{D.8})$$

and then

$$S = \frac{Na^{N+1}}{a-1} - \frac{a(a^N - 1)}{(a-1)^2}. \quad (\text{D.9})$$

Substituting $a = e^{i\beta\pi}$,

$$S = \frac{Ne^{i\beta\pi(N+1)}}{e^{i\beta\pi} - 1} - \frac{e^{i\beta\pi}(e^{i\beta\pi N} - 1)}{(e^{i\beta\pi} - 1)^2}. \quad (\text{D.10})$$

Knowing that $e^{ix} + e^{-ix} = 2\cos x$,

$$S = \frac{Ne^{i\beta\pi(N+1)}}{e^{\frac{i\beta\pi}{2}}(e^{\frac{i\beta\pi}{2}} - e^{-\frac{i\beta\pi}{2}})} - \frac{e^{i\beta\pi}(e^{i\beta\pi N} - 1)}{(e^{\frac{i\beta\pi}{2}}(e^{\frac{i\beta\pi}{2}} - e^{-\frac{i\beta\pi}{2}}))^2}. \quad (\text{D.11})$$

Thus,

$$S = \frac{Ne^{i\beta\pi(N+1)}e^{-\frac{i\beta\pi}{2}}}{(e^{\frac{i\beta\pi}{2}} - e^{-\frac{i\beta\pi}{2}})} - \frac{e^{i\beta\pi}(e^{i\beta\pi N} - 1)}{e^{i\beta\pi}(e^{\frac{i\beta\pi}{2}} - e^{-\frac{i\beta\pi}{2}})^2}, \quad (\text{D.12})$$

and going back to trigonometric notation,

$$S = \frac{N(\cos((N+1/2)\beta\pi) + i\sin((N+1/2)\beta\pi))}{2i\sin(\beta\pi/2)} - \frac{\cos(N\beta\pi) + i\sin(N\beta\pi) - 1}{(2i\sin(\beta\pi/2))^2}. \quad (\text{D.13})$$

Real and imaginary parts can be separated as

$$S = \frac{N\sin((N+1/2)\beta\pi)}{2\sin(\beta\pi/2)} + \frac{\cos(N\beta\pi) - 1}{4\sin^2(\beta\pi/2)} + i\left(\frac{\sin(N\beta\pi)}{4\sin^2(\beta\pi/2)} - \frac{N\cos((N+1/2)\beta\pi)}{2\sin(\beta\pi/2)}\right) \quad (\text{D.14})$$

where the imaginary part corresponds to the result of equation D by setting $N = j-1$, so

$$\sum_{k=1}^{j-1} k\sin(k\beta\pi) = \frac{\sin((j-1)\beta\pi)}{4\sin^2(\beta\pi/2)} - \frac{(j-1)\cos((j-1/2)\beta\pi)}{2\sin(\beta\pi/2)}. \quad (\text{D.15})$$

Some trigonometric identities then yield equation 5.28.

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