Complex frequency band structure of periodic thermo-diffusive materials by Floquet–Bloch theory

1 Introduction

The advances in different engineering fields, involving, among others, structural monitoring, nano-medicine, military–aerospace industries and wearable electronics, call for the need of composite materials with increasingly improved performances. Optimized responses in terms of toughness, strength, mass diffusivity, thermal conductivity or also electric permittivity can indeed be obtained by properly combining materials characterized by different physical properties. In the framework of renewable energy applications, multi-phase materials have been widely adopted especially in the manufacturing of battery devices, such as solid oxide fuel cells (SOFCs) [21,31,42] and lithium ion batteries [22,24,52]. In particular, SOFCs are electrochemical devices able to convert the chemical energy originally stored in a fuel into electrical power. Such fuel cells are characterized by very high energy conversion performance and are extremely eligible for realizing efficient small-scale power generation systems, with an efficiency up to 60%. The typical SOFC building block, schematized in Fig. 1, consists of a layer of doped ceramic material, used as electrolyte, that is sandwiched between two heat-resistant electrodes, i.e. cathode and anode, made of porous materials [16]. The working principle of SOFC devices can be described as follows. The cathode is supplied with both oxygen, as oxidant material, and electrons that are provided by an external circuit. At this point, a chemical reaction takes place and oxygen ions are released. These ions migrate into the electrolyte towards the anode, on which they combine with the H₂ fuel, forming
water and electrons. These electrons travel along the circuit, generating an electrical current. The single cell comprised of anode, electrolyte and cathode is provided with an interconnect separator and flow channels on each side. A number of cells are typically stacked together, working in series, in order to build up the voltage for the power generating capacity required in practical uses. The resulting composite material is, thus, periodic.

The strengths of SOFCs are the great flexibility in sizing and nearly zero emissions [37], while the weaknesses concern both the very high operating temperature involved, usually in the range 60–1000 °C, and the intense particle flows. As a result, these devices typically undergo severe stresses induced by coupled chemothermo-mechanical phenomena, thus also influencing the choice of the materials adopted in their manufacturing [48,51].

A comprehensive understanding of the SOFC functioning cannot disregard the strong mutual influence between the macroscopic behaviour of the thermo-diffusive composite materials and the multi-physics phenomena taking place at the scale of the constituents [16,31]. In this context, multi-scale techniques are powerful tools to gather global constitutive information starting from the detailed description of the microscopic material scale. In particular, various homogenization approaches, including computational and asymptotic strategies, have been proposed for investigating the overall elastic properties of composite materials with periodic microstructures, both in the static [3–6,8,9,13,14,18,27,29] and in the dynamic regimes [7,17,60]. Examples of multi-physics homogenization approaches range from thermo-elastic [2,26,35,38,65], to piezoelectric and thermo-piezoelectric problems [19,20,25,28], up to thermo-diffusive phenomena [10–12,54].

Standard homogenization approaches, nevertheless, show some inner limitations in the study of high-frequency dispersive waves characterized by short wavelengths. In such cases, it can be useful resorting to micromechanical approaches [1,32,33,55,61]. More specifically, in the framework of thermo-elastic problems, different approaches have been proposed in the literature. On the one hand, classical dynamic thermo-elasticity approaches deal with the Fourier law, directly leading to parabolic heat conduction field equations coupled with the hyperbolic field equations describing the elasto-mechanical problem [15,23,36,40,43]. On the other hand, generalized dynamic theory of thermo-elasticity have been proposed. Among others, the Maxwell–Cattaneo law is used, as an alternative to the Fourier law, so that the resulting coupled field equations are both hyperbolic [32,33,39,41,59].

With specific reference to thermo-diffusive problems, [56] investigated the plane harmonic elasto-thermo-diffusive waves in semiconductors. Besides the shear waves decoupled from to other fields, coupled longitudinal waves are observed in an infinite semiconductor. In [57], the propagation of elasto-thermo-diffusive surface waves in an homogeneous and isotropic semiconductor material half-space, with relaxation of heat and charge carrier fields, is performed. [58] studied the propagation of elasto-thermo-diffusive surface (Rayleigh) waves under the effect of thermal field in a semiconductor half-space underlying a viscous or inviscid fluid half-space.
or layer of finite thickness with varying temperature. It emerged that the phase velocity and the attenuation coefficient of the Rayleigh waves are strongly influenced by a set of parameters defining the fluid loading. Moreover, in [10] the authors investigate the influence of the temperature variation on the overall elastic and inertial properties of SOFCs-like fuel cells. The Floquet–Bloch spectrum, related to the propagation of acoustic waves in these devices, is also determined and discussed in detail.

In this work, the focus is on a micromechanical dynamical study of SOFCs-like cells, taking into account the coupling between thermal, mechanical and diffusive phenomena. In this framework, we are interested in investigating the possible influence that the interaction between such phenomena might have on the dispersive free waves propagation within a linear elastic periodic material. To this aim, the frequency band structure of such devices is determined and critically analysed. With this in mind, we consider the governing equations of the coupled problem, based on the Fourier law of heat conduction and the Fick law of diffusion [44–47,49,50], and apply the Floquet–Bloch theory. In particular, by exploiting both bilateral Laplace transforms in time and Fourier transforms in space, we obtain an infinite algebraic linear system in terms of complex frequencies and wave vectors. Such a resulting system admits eigenvalues representing the complex spectrum of the periodic material. An accurate numerical solution can be found by truncating the infinite system at a given finite number of considered equations, determined on the basis of a properly conceived convergence analysis. In this context, regularization techniques are useful to smooth the results in terms of constitutive components that can be affected by the Gibbs phenomenon, that is, oscillations particularly pronounced near the discontinuities between materials phases in the periodic cells. Finally, after performing a discretization of the wave vector space, a finite sequence of eigenvalue problems is obtained, whose solutions are the complex angular frequencies corresponding to a given wave vector.

The paper is organized as follows. In Sect. 2, the governing equations of the periodic thermo-diffusive material, considered as a first-order continuum, are recalled. By exploiting the periodicity of the medium, the Christoffel equations are complemented by the Floquet–Bloch boundary conditions. Section 3 is devoted to the determination of the infinite algebraic system, characterizing the propagation of damped Bloch waves. Moreover, in Sect. 4 the generalized infinite eigenvalue problem is truncated and the approximate solution of the Floquet–Bloch spectrum is found. Section 5 presents numerical examples focused on the study of damped wave propagation in SOFC-like devices. Finally, some concluding remarks are summarized in Sect. 6.

2 Governing equations of periodic elastic thermo-diffusive first-order continuum

Let us consider a periodic elastic heterogeneous material undergoing thermo-diffusive phenomena. Restricting our analysis to the two-dimensional case, we adopt a linear elastic thermo-diffusive first-order continuum to model each material phase of the heterogeneous medium schematically shown in Fig. 1a. Given the medium periodicity, it is possible to identify the periodic cell \( A = [0, d_1] \times [0, d_2] \) in Fig. 1b, characterized by two orthogonal vectors of periodicity \( v_1 = d_1 e_1, v_2 = d_2 e_2 \), with \( e_1 \) and \( e_2 \) being a given orthogonal base.

Each material point \( x = x_1 e_1 + x_2 e_2 \) is endowed with a displacement field \( u(x, t) = u_i e_i \) and a relative temperature field \( \dot{\theta}(x, t) = T(x, t) - T_0 \), where \( T(x, t) \) is the absolute temperature, \( T_0 \) is a reference stress-free temperature and \( \eta(x, t) \) is a chemical potential field. The coupled constitutive relations link the stress tensor \( \sigma(x, t) = \sigma_{ij} e_i \otimes e_j \), the heat and mass fluxes \( q(x, t) = q_i e_i \) and \( j(x, t) = j_i e_i \), respectively, to the aforementioned relevant fields \( u(x), \dot{\theta}(x) \) and \( \eta(x) \), that is,

\[
\sigma(x, t) = C(x) \nabla u(x, t) - \alpha(x) \dot{\theta}(x, t) - \beta(x) \eta(x, t),
\]

\[
q(x, t) = -K(x) \nabla \dot{\theta}(x, t),
\]

\[
j(x, t) = -D(x) \nabla \eta(x, t),
\]

where \( C = C_{ijkl} e_i \otimes e_j \otimes e_k \otimes e_l \) is the fourth-order elastic tensor with major and minor symmetries, \( K = K_{ij} e_i \otimes e_j \) is the symmetric second-order heat conduction tensor, \( D = D_{ij} e_i \otimes e_j \) is the symmetric second-order mass diffusion tensor, \( \alpha = \alpha_{ij} e_i \otimes e_j \) is the symmetric second-order thermal dilatation tensor and \( \beta = \beta_{ij} e_i \otimes e_j \) is the symmetric second-order diffusive expansion tensor.

The following balance equations hold:

\[
\nabla \cdot \sigma(x, t) + f(x, t) = \rho(x) \ddot{u}(x, t),
\]

\[
-\nabla \cdot q(x, t) + \ddot{\theta}(x, t) = \ddot{\rho}(x) \dot{\theta}(x, t) + T_0 \alpha(x) : \nabla \dot{u}(x, t) + T_0 \Psi(x) \dot{j}(x, t),
\]

\[
-\nabla \cdot j(x, t) + s(x, t) = c(x) \dot{\eta}(x, t) + \beta(x) : \nabla \dot{u}(x, t) + \Psi(x) \dot{\theta}(x, t),
\]
with \( f = f_j e_j \) being the body forces, \( \dot{r} \) the heat source, \( s \) the mass source, \( \rho \) the mass density, \( \bar{p} \) and \( c \) material constants (the former is related to the specific heat at constant strain and to thermo-diffusive effects, while the latter is related to diffusive effects) and \( \Psi \) a thermo-diffusive coupling constant.

According to [44–46], the governing equations are finally obtained by plugging the constitutive equations into the balance equations that take the form

\[
\nabla \cdot (C \nabla u(x, t) - \alpha \frac{\partial u}{\partial x} - \beta \eta(x, t)) + f(x, t) = \rho \dot{u}(x, t),
\]

\[
\nabla \cdot (K \nabla \dot{\vartheta}(x, t)) = \nabla \cdot (\Psi \dot{\eta}(x, t) + r(x, t)) + \rho \dot{\vartheta}(x, t),
\]

\[
\nabla \cdot (D \nabla \dot{\eta}(x, t)) - \beta \dot{\vartheta}(x, t) + c \dot{\eta}(x, t) = 0,
\]

where the meaning of the symbols introduced in (8) is \( K = \tilde{K}/T_0, r = \tilde{r}/T_0 \) and \( p = \tilde{p}/T_0 \).

Since we focus on periodic materials, the constitutive tensors involved in Eqs. (7), (8) and (9) satisfy periodicity conditions within the periodic cell, i.e. \( \forall x \in A \). This means that the elastic tensor, the heat conduction and the mass diffusion tensors are characterized by \( A \)-periodicity, that is,

\[
C(x + v_i) = C(x),
\]

\[
K(x + v_i) = K(x),
\]

\[
D(x + v_i) = D(x).
\]

Similarly, the inertial terms result in

\[
\rho(x + v_i) = \rho(x),
\]

\[
\rho(x + v_i) = \rho(x),
\]

\[
c(x + v_i) = c(x),
\]

and, finally, the thermal dilatation tensor, the diffusive expansion tensor and the thermo-diffusive coupling constant comply with the following relations:

\[
\alpha(x + v_i) = \alpha(x),
\]

\[
\beta(x + v_i) = \beta(x),
\]

\[
\Psi(x + v_i) = \Psi(x).
\]

We focus the attention on the study of wave propagation in the thermo-diffusive periodic material. Note that, due to the structure of the governing equations (7)–(9), the waves propagating in the medium are in general dispersive and characterized by temporal damping. To this aim, we apply the time bilateral Laplace transform to Eqs. (4)–(6) in the case of zero source terms, i.e. \( f = 0, r = 0, s = 0 \). We recall that the time bilateral Laplace transform, or Fourier transform with complex argument [62,64], of a given a function \( g(x, t) \), is defined as

\[
L_t \left[ g(x, t) \right] = \int_{-\infty}^{+\infty} g(x, t) e^{-I \omega t} dt = \hat{g}(x),
\]

where \( \omega \) is the complex angular frequency (\( \omega \in \mathbb{C} \)) and \( I \) is the imaginary unit, with \( I^2 = -1 \). It follows that the governing equations in the transformed space, also referred to as generalized Christoffel equations, are

\[
\nabla \cdot (\nabla \hat{u} - \alpha \dot{\vartheta} - \nabla \beta \dot{\eta}) + \rho \omega^2 \hat{u} = 0,
\]

\[
\nabla \cdot (K \nabla \dot{\vartheta}) - I \omega \left( \alpha : \nabla \hat{u} + \Psi \dot{\eta} + p \dot{\vartheta} \right) = 0,
\]

\[
\nabla \cdot (D \nabla \dot{\eta}) - I \omega \left( \beta : \nabla \hat{u} + \Psi \dot{\eta} + c \dot{\eta} \right) = 0,
\]

where \( \hat{u}, \dot{\vartheta} \) and \( \dot{\eta} \) are the bilateral Laplace transforms of the displacement field, the temperature field and the chemical potential field, respectively.

By exploiting the periodicity of the medium, it is possible to analyse the generalized Christoffel equations (20), (21) and (22) in the periodic cell \( A \) undergoing the Floquet–Bloch boundary conditions. Let \( k = k_1 e_1 + k_2 e_2 \in B \) be the wave vector, being \( k_1, k_2 \) the wave numbers and \( B = [-\pi/d_1, \pi/d_1] \times [-\pi/d_2, \pi/d_2] \) the
first Brillouin zone related to the periodic cell with orthogonal periodicity vectors. Moreover, it is possible to define the unit vector of propagation \( \mathbf{m} = k/||k|| \). The Floquet–Bloch boundary conditions read

\[
\hat{u}(x + v_p) = e^{i(k \cdot v_p)} \hat{u}(x), \\
\hat{\theta}(x + v_p) = e^{i(k \cdot v_p)} \hat{\theta}(x), \\
\hat{\eta}(x + v_p) = e^{i(k \cdot v_p)} \hat{\eta}(x),
\]

where \( v_p \) is the periodicity vector \((p = 1, 2)\), \( n_h \) is the outward normal unit vector \((h = 1, 2)\) and \( \hat{\sigma}, \hat{q} \) and \( \hat{j} \) are the bilateral Laplace transforms of the stress tensor, heat and mass fluxes, respectively. It is worth noting that by adopting the constitutive relations, the following expressions hold:

\[
\hat{\sigma} = C \nabla \hat{u} - \alpha \hat{\theta} - \beta \hat{\eta}, \\
\hat{q} = -K \nabla \hat{\theta}, \\
\hat{j} = -D \nabla \hat{\eta}.
\]

3 Damped Bloch wave propagation and Floquet–Bloch spectrum

In accordance with the Floquet–Bloch theory, here generalized to the case of an elastic thermo-diffusive medium, we resort to the Floquet–Bloch decomposition, that is,

\[
\hat{u}(x) = \tilde{u}(x) e^{i(k \cdot x)}, \\
\hat{\theta}(x) = \tilde{\theta}(x) e^{i(k \cdot x)}, \\
\hat{\eta}(x) = \tilde{\eta}(x) e^{i(k \cdot x)},
\]

with \( \tilde{u}(x), \tilde{\theta}(x), \tilde{\eta}(x) \) being the \( A \)-periodic Bloch amplitudes of the displacement, temperature and chemical potential fields, in the transformed space. It is worth noting that Eqs. (32)–(34) automatically satisfy the Floquet–Bloch boundary conditions (23)–(28).

By plugging in Eqs. (32)–(34) into Eqs. (20)–(22), the generalized Christoffel equations take the following form:

\[
\begin{align*}
\nabla \cdot \left( C (x) \nabla \left( \tilde{u}(x) e^{i(k \cdot x)} \right) \right) - \nabla \cdot \left( \alpha (x) \tilde{\theta}(x) e^{i(k \cdot x)} \right) \\
- \nabla \cdot \left( \beta (x) \tilde{\eta}(x) e^{i(k \cdot x)} \right) + \rho (x) \omega^2 \tilde{u}(x) e^{i(k \cdot x)} = 0, \\
\n\nabla \cdot \left( K (x) \nabla \left( \tilde{\theta}(x) e^{i(k \cdot x)} \right) \right) - I \omega \alpha (x) : \nabla \left( \tilde{u}(x) e^{i(k \cdot x)} \right) \\
- I \omega \beta (x) : \nabla \left( \tilde{\eta}(x) e^{i(k \cdot x)} \right) + \rho (x) \omega^2 \tilde{u}(x) e^{i(k \cdot x)} = 0, \\
\n\n\nabla \cdot \left( D (x) \nabla \left( \tilde{\eta}(x) e^{i(k \cdot x)} \right) \right) - I \omega \beta (x) : \nabla \left( \tilde{u}(x) e^{i(k \cdot x)} \right) \\
- I \omega \alpha (x) : \nabla \left( \tilde{\theta}(x) e^{i(k \cdot x)} \right) + \rho (x) \omega^2 \tilde{u}(x) e^{i(k \cdot x)} = 0.
\end{align*}
\]

The governing equations (35)–(37) can be properly manipulated by performing the space Fourier transform, which for a generic function \( g(x) \) is defined as

\[
F_x \left[ g(x) \right] = \int_{\mathbb{R}^2} g(x) e^{-ir \cdot x} dx,
\]

where \( r \) is a vector in the transformed space of wave vectors, with \( r \in \mathbf{B} \). It follows that in transformed space and frequency domain, Eqs. (35)–(37) in component form become
where * denotes the convolution product symbol.

By performing the convolution products in Eqs. (39)–(41), after some manipulations described in Appendix A, we obtain

\[
\begin{align*}
-4\pi^2 r_j & \int_{\mathbb{R}^2} q_k \mathcal{F}_x[C_{ijkl}] (r - q) \mathcal{F}_x[\bar{u}_k] (q - k) \, dq - 4\pi^2 i r_j \int_{\mathbb{R}^2} \mathcal{F}_x[\alpha_{ij}] (r - q) \mathcal{F}_x[\bar{\beta}] (q - k) \, dq \\
-4\pi^2 i r_j & \int_{\mathbb{R}^2} \mathcal{F}_x[\beta_{ij}] (r - q) \mathcal{F}_x[\bar{\eta}] (q - k) \, dq + 4\pi^2 \omega^2 \int_{\mathbb{R}^2} \mathcal{F}_x[\rho] (r - q) \mathcal{F}_x[\bar{u}_i] (q - k) \, dq = 0,
\end{align*}
\]

(42)

\[
\begin{align*}
-4\pi^2 r_i & \int_{\mathbb{R}^2} q_j \mathcal{F}_x[K_{ijkl}] (r - q) \mathcal{F}_x[\bar{\beta}] (q - k) \, dq + 4\pi^2 \omega \int_{\mathbb{R}^2} q_j \mathcal{F}_x[\alpha_{ij}] (r - q) \mathcal{F}_x[\bar{u}_i] (q - k) \, dq \\
-4\pi^2 i \omega & \int_{\mathbb{R}^2} \mathcal{F}_x[\psi] (r - q) \mathcal{F}_x[\bar{\eta}] (q - k) \, dq - 4\pi^2 i \omega \int_{\mathbb{R}^2} \mathcal{F}_x[\rho] (r - q) \mathcal{F}_x[\bar{\beta}] (q - k) \, dq = 0,
\end{align*}
\]

(43)

\[
\begin{align*}
-4\pi^2 r_i & \int_{\mathbb{R}^2} q_j \mathcal{F}_x[D_{ijkl}] (r - q) \mathcal{F}_x[\bar{\eta}] (q - k) \, dq + 4\pi^2 \omega \int_{\mathbb{R}^2} q_j \mathcal{F}_x[\beta_{ij}] (q) \mathcal{F}_x[\bar{u}_i] (q - k) \, dq \\
-4\pi^2 i \omega & \int_{\mathbb{R}^2} \mathcal{F}_x[\psi] (r - q) \mathcal{F}_x[\bar{\eta}] (q - k) \, dq - 4\pi^2 i \omega \int_{\mathbb{R}^2} \mathcal{F}_x[c] (r - q) \mathcal{F}_x[\bar{\eta}] (q - k) \, dq = 0,
\end{align*}
\]

(44)

with \(q \in \mathbb{B}\). Moreover, by exploiting the \(A\)-periodicity of the constitutive tensors, (10)–(12), (16)–(18), of the inertial terms (13)–(15) and of the unknown Bloch amplitudes \(\bar{u}(x)\), \(\bar{\beta}(x)\) and \(\bar{\eta}(x)\), their Fourier transforms take the form of weighted Dirac combs, whose weights are the related Fourier coefficients. It is worth noting that while the Fourier coefficients associated with the constitutive tensors and inertial terms are fully determined, those associated with the functions \(\bar{u}(x)\), \(\bar{\beta}(x)\) and \(\bar{\eta}(x)\) are unknowns. In particular, we first introduce the vector

\[
\pi_d = \left(\frac{2\pi}{d_1}, \frac{2\pi}{d_2}\right) \in \mathbb{R}^2,
\]

(45)

together with the two generic vectors \(\mathbf{m}\) and \(\mathbf{n}\) with integer components

\[
\mathbf{m} = (m_1, m_2) \in \mathbb{Z}^2,
\]

(46)

\[
\mathbf{n} = (n_1, n_2) \in \mathbb{Z}^2,
\]

(47)

and we exploit the Hadamard product as

\[
\pi_d \circ \mathbf{m} = \left(\frac{2\pi}{d_1} m_1, \frac{2\pi}{d_2} m_2\right),
\]

(48)

\[
\pi_d \circ \mathbf{n} = \left(\frac{2\pi}{d_1} n_1, \frac{2\pi}{d_2} n_2\right).
\]

(49)
It follows that Eqs. (42)–(44) can be specialized as

\[
-4\pi^2 r_j \int_{\mathbb{R}^2} q_k \sum_{m \in \mathbb{Z}^2} C_{i j h k}^{m_1 m_2} \delta (r - q - \pi d \circ m) \sum_{n \in \mathbb{Z}^2} \bar{a}_{i j n h}^{m_1 n_2} \delta (q - k - \pi d \circ n) \, dq
\]

\[
-4\pi^2 I r_j \int_{\mathbb{R}^2} \sum_{m \in \mathbb{Z}^2} \alpha_{i j h k}^{m_1 m_2} \delta (r - q - \pi d \circ m) \sum_{n \in \mathbb{Z}^2} \bar{b}_{i j n h}^{m_1 n_2} \delta (q - k - \pi d \circ n) \, dq
\]

\[
-4\pi^2 I r_j \int_{\mathbb{R}^2} \sum_{m \in \mathbb{Z}^2} \beta_{i j h k}^{m_1 m_2} \delta (r - q - \pi d \circ m) \sum_{n \in \mathbb{Z}^2} \bar{c}_{i j n h}^{m_1 n_2} \delta (q - k - \pi d \circ n) \, dq
\]

\[
+4\pi^2 \omega^2 \int_{\mathbb{R}^2} \sum_{m \in \mathbb{Z}^2} \rho_{i j h k}^{m_1 m_2} \delta (r - q - \pi d \circ m) \sum_{n \in \mathbb{Z}^2} \bar{d}_{i j n h}^{m_1 n_2} \delta (q - k - \pi d \circ n) \, dq = 0, \quad (50)
\]

\[
-4\pi^2 r_i \int_{\mathbb{R}^2} q_j \sum_{m \in \mathbb{Z}^2} K_{i j h k}^{m_1 m_2} \delta (r - q - \pi d \circ m) \sum_{n \in \mathbb{Z}^2} \bar{e}_{i j n h}^{m_1 n_2} \delta (q - k - \pi d \circ n) \, dq
\]

\[
+4\pi^2 \omega \int_{\mathbb{R}^2} q_j \sum_{m \in \mathbb{Z}^2} \alpha_{i j h k}^{m_1 m_2} \delta (r - q - \pi d \circ m) \sum_{n \in \mathbb{Z}^2} \bar{f}_{i j n h}^{m_1 n_2} \delta (q - k - \pi d \circ n) \, dq
\]

\[
-4\pi^2 I \omega \int_{\mathbb{R}^2} \sum_{m \in \mathbb{Z}^2} \psi_{i j h k}^{m_1 m_2} \delta (r - q - \pi d \circ m) \sum_{n \in \mathbb{Z}^2} \bar{g}_{i j n h}^{m_1 n_2} \delta (q - k - \pi d \circ n) \, dq
\]

\[
-4\pi^2 I \omega \int_{\mathbb{R}^2} \sum_{m \in \mathbb{Z}^2} \rho_{i j h k}^{m_1 m_2} \delta (r - q - \pi d \circ m) \sum_{n \in \mathbb{Z}^2} \bar{h}_{i j n h}^{m_1 n_2} \delta (q - k - \pi d \circ n) \, dq
\]

\[
-4\pi^2 I \omega \int_{\mathbb{R}^2} \sum_{m \in \mathbb{Z}^2} c_{i j h k}^{m_1 m_2} \delta (r - q - \pi d \circ m) \sum_{n \in \mathbb{Z}^2} \bar{i}_{i j n h}^{m_1 n_2} \delta (q - k - \pi d \circ n) \, dq = 0, \quad (51)
\]

where \( \delta (\cdot) \) denotes the Dirac-delta generalized function, \( C_{i j h k}^{m_1 m_2}, K_{i j h k}^{m_1 m_2}, D_{i j h k}^{m_1 m_2}, \alpha_{i j h k}^{m_1 m_2}, \beta_{i j h k}^{m_1 m_2}, \psi_{i j h k}^{m_1 m_2}, \rho_{i j h k}^{m_1 m_2}, \) \( p_{i j h k}^{m_1 m_2}, c_{i j h k}^{m_1 m_2} \) are the weights of the Dirac combs associated with the constitutive tensors and the inertial terms, and \( \bar{u}_{i j n h}^{m_1 n_2}, \bar{b}_{i j n h}^{m_1 n_2}, \bar{c}_{i j n h}^{m_1 n_2} \) are the weights of the Dirac combs associated with the unknown Bloch amplitudes.

By recalling the property \( g(r) \delta (r - r_0) = g(r_0) \delta (r - r_0) \) which applies to a generic smooth function \( g(r) \) and a constant vector \( r_0 \), and by computing the integrals in (50)–(52), we obtain

\[
-4\pi^2 \sum_{m, n \in \mathbb{Z}^2} \left( k_j + \frac{2\pi (m_j + n_j)}{d_j} \right) \left( k_k + \frac{2\pi n_k}{d_k} \right) c_{i j h k}^{m_1 m_2} \bar{u}_{i j n h}^{m_1 n_2} \delta (r - k - \pi d \circ (m + n))
\]

\[
-4\pi^2 I \sum_{m, n \in \mathbb{Z}^2} \left( k_j + \frac{2\pi (m_j + n_j)}{d_j} \right) \alpha_{i j h k}^{m_1 m_2} \bar{b}_{i j n h}^{m_1 n_2} \delta (r - k - \pi d \circ (m + n))
\]

\[
-4\pi^2 I \sum_{m, n \in \mathbb{Z}^2} \left( k_j + \frac{2\pi (m_j + n_j)}{d_j} \right) \beta_{i j h k}^{m_1 m_2} \bar{c}_{i j n h}^{m_1 n_2} \delta (r - k - \pi d \circ (m + n))
\]

\[
+4\pi^2 \omega^2 \sum_{m, n \in \mathbb{Z}^2} \rho_{i j h k}^{m_1 m_2} \bar{d}_{i j n h}^{m_1 n_2} \delta (r - k - \pi d \circ (m + n)) = 0, \quad (53)
\]
\[-4\pi^2 \sum_{m,n \in \mathbb{Z}^2} \left( k_i + \frac{2\pi (m_i + n_i)}{d_i} \right) \left( k_j + \frac{2\pi n_j}{d_j} \right) K_{ij}^{m_1 n_2} \tilde{\eta}^{n_1 n_2} \delta \left( r - \mathbf{k} - \mathbf{\pi}_d \circ (m + n) \right) \]

\[+ 4\pi^2 \omega \sum_{m,n \in \mathbb{Z}^2} \left( k_j + \frac{2\pi n_j}{d_j} \right) \alpha_{ij}^{m_2} \tilde{u}_{i}^{n_1 n_2} \delta \left( r - \mathbf{k} - \mathbf{\pi}_d \circ (m + n) \right) \]

\[+ 4\pi^2 I \omega \sum_{m,n \in \mathbb{Z}^2} \psi^{m_1 m_2} \tilde{\eta}^{n_1 n_2} \delta \left( r - \mathbf{k} - \mathbf{\pi}_d \circ (m + n) \right) \]

\[+ 4\pi^2 \omega \sum_{m,n \in \mathbb{Z}^2} \left( k_j + \frac{2\pi n_j}{d_j} \right) \beta_{ij}^{m_2} \tilde{u}_{i}^{n_1 n_2} \delta \left( r - \mathbf{k} - \mathbf{\pi}_d \circ (m + n) \right) \]

\[- 4\pi^2 I \omega \sum_{m,n \in \mathbb{Z}^2} \phi^{m_1 m_2} \tilde{\eta}^{n_1 n_2} \delta \left( r - \mathbf{k} - \mathbf{\pi}_d \circ (m + n) \right) \]

\[- 4\pi^2 I \omega \sum_{m,n \in \mathbb{Z}^2} c^{m_1 m_2} \tilde{\eta}^{n_1 n_2} \delta \left( r - \mathbf{k} - \mathbf{\pi}_d \circ (m + n) \right) = 0. \] (54)

Moreover, by defining the following vectors with integer components:

\[\tilde{r} = m + n \in \mathbb{Z}^2, \]

\[\tilde{q} = m \in \mathbb{Z}^2, \] (56) (57)

Eqs. (53)–(55) become

\[- 4\pi^2 \sum_{\tilde{r} \in \mathbb{Z}^2} \left[ \left( k_j + \frac{2\pi \tilde{r}_j}{d_j} \right) \sum_{\tilde{q} \in \mathbb{Z}^2} \left( k_k + \frac{2\pi \tilde{q}_k}{d_k} \right) c^{\tilde{r}_1,\tilde{r}_2,\tilde{r}_3} \tilde{\eta}^{q_1 q_2 q_3} \right] \delta \left( r - \mathbf{k} - \mathbf{\pi}_d \circ \tilde{r} \right) \]

\[+ 4\pi^2 I \sum_{\tilde{r} \in \mathbb{Z}^2} \left[ \left( k_j + \frac{2\pi \tilde{r}_j}{d_j} \right) \sum_{\tilde{q} \in \mathbb{Z}^2} \alpha_{ij}^{\tilde{r}_1,\tilde{r}_2,\tilde{r}_3,\tilde{q}_1,\tilde{q}_2} \right] \delta \left( r - \mathbf{k} - \mathbf{\pi}_d \circ \tilde{r} \right) \]

\[+ 4\pi^2 I \sum_{\tilde{r} \in \mathbb{Z}^2} \left[ \left( k_j + \frac{2\pi \tilde{r}_j}{d_j} \right) \sum_{\tilde{q} \in \mathbb{Z}^2} \beta_{ij}^{\tilde{r}_1,\tilde{r}_2,\tilde{r}_3,\tilde{q}_1,\tilde{q}_2} \right] \delta \left( r - \mathbf{k} - \mathbf{\pi}_d \circ \tilde{r} \right) \]

\[+ 4\pi^2 \omega^2 \sum_{\tilde{r} \in \mathbb{Z}^2} \sum_{\tilde{q} \in \mathbb{Z}^2} \rho^{\tilde{r}_1,\tilde{r}_2,\tilde{r}_3,\tilde{q}_1,\tilde{q}_2} \delta \left( r - \mathbf{k} - \mathbf{\pi}_d \circ \tilde{r} \right) = 0. \] (58)

\[- 4\pi^2 \sum_{\tilde{r} \in \mathbb{Z}^2} \left[ \left( k_i + \frac{2\pi \tilde{r}_i}{d_i} \right) \sum_{\tilde{q} \in \mathbb{Z}^2} \left( k_j + \frac{2\pi \tilde{q}_j}{d_j} \right) K_{ij}^{\tilde{r}_1,\tilde{r}_2,\tilde{r}_3,\tilde{q}_1,\tilde{q}_2} \right] \delta \left( r - \mathbf{k} - \mathbf{\pi}_d \circ \tilde{r} \right) \]

\[+ 4\pi^2 \omega \sum_{\tilde{r} \in \mathbb{Z}^2} \sum_{\tilde{q} \in \mathbb{Z}^2} \left( k_j + \frac{2\pi \tilde{q}_j}{d_j} \right) \alpha_{ij}^{\tilde{r}_1,\tilde{r}_2,\tilde{r}_3,\tilde{q}_1,\tilde{q}_2} \delta \left( r - \mathbf{k} - \mathbf{\pi}_d \circ \tilde{r} \right) \]

\[- 4\pi^2 I \omega \sum_{\tilde{r} \in \mathbb{Z}^2} \sum_{\tilde{q} \in \mathbb{Z}^2} \psi^{\tilde{r}_1,\tilde{r}_2,\tilde{r}_3,\tilde{q}_1,\tilde{q}_2} \delta \left( r - \mathbf{k} - \mathbf{\pi}_d \circ \tilde{r} \right) \]
\[-4\pi^2 I \omega \sum_{\mathbf{r} \in \mathbb{Z}^2} \left[ \sum_{\mathbf{q} \in \mathbb{Z}^2} p^{\bar{r}_1 - \bar{q}_1} r_2 - \bar{q}_2 \bar{q}_1 \bar{q}_2 \right] \delta (\mathbf{r} - \mathbf{k} - \mathbf{\pi}_d \circ \bar{\mathbf{r}}) = 0, \] 
\[-4\pi^2 \sum_{\mathbf{r} \in \mathbb{Z}^2} \left[ \left( k_i + \frac{2\pi \bar{r}_j}{d_i} \right) \sum_{\mathbf{q} \in \mathbb{Z}^2} \left( k_j + \frac{2\pi \bar{q}_j}{d_j} \right) \beta^{\bar{r}_1 - \bar{q}_1} r_2 - \bar{q}_2 \bar{q}_1 \bar{q}_2 \right] \delta (\mathbf{r} - \mathbf{k} - \mathbf{\pi}_d \circ \bar{\mathbf{r}}) \] 
\[+ 4\pi^2 \omega \sum_{\mathbf{r} \in \mathbb{Z}^2} \left[ \sum_{\mathbf{q} \in \mathbb{Z}^2} \left( k_j + \frac{2\pi \bar{q}_j}{d_j} \right) \rho^{\bar{r}_1 - \bar{q}_1} r_2 - \bar{q}_2 \bar{q}_1 \bar{q}_2 \right] \delta (\mathbf{r} - \mathbf{k} - \mathbf{\pi}_d \circ \bar{\mathbf{r}}) \] 
\[-4\pi^2 I \omega \sum_{\mathbf{r} \in \mathbb{Z}^2} \left[ \sum_{\mathbf{q} \in \mathbb{Z}^2} \psi^{\bar{r}_1 - \bar{q}_1} r_2 - \bar{q}_2 \bar{q}_1 \bar{q}_2 \right] \delta (\mathbf{r} - \mathbf{k} - \mathbf{\pi}_d \circ \bar{\mathbf{r}}) \] 
\[-4\pi^2 I \omega \sum_{\mathbf{r} \in \mathbb{Z}^2} \left[ \sum_{\mathbf{q} \in \mathbb{Z}^2} c^{\bar{r}_1 - \bar{q}_1} r_2 - \bar{q}_2 \bar{q}_1 \bar{q}_2 \right] \delta (\mathbf{r} - \mathbf{k} - \mathbf{\pi}_d \circ \bar{\mathbf{r}}) = 0. \] 

Note that Eqs. (58)–(60) are weighted Dirac combs set equal to zero. Therefore, the summation of all the weights associated with the Dirac-delta generalized function \( \delta (\mathbf{r} - \mathbf{k} - \mathbf{\pi}_d \circ \bar{\mathbf{r}}) \) must vanish, for each \( \mathbf{r} \in \mathbb{Z}^2 \).

This produces the following generalized eigenvalue problem, expressed as an infinite algebraic linear system:

\[- \left( \frac{2\pi \bar{r}_j}{d_j} + k_j \right) \sum_{\mathbf{q} \in \mathbb{Z}^2} \left( \frac{2\pi \bar{q}_k}{d_k} + k_k \right) C^{\bar{r}_1 - \bar{q}_1} r_2 - \bar{q}_2 \bar{q}_1 \bar{q}_2 - I \left( \frac{2\pi \bar{r}_j}{d_j} + k_j \right) \sum_{\mathbf{q} \in \mathbb{Z}^2} \alpha^{\bar{r}_1 - \bar{q}_1} r_2 - \bar{q}_2 \bar{q}_1 \bar{q}_2 = 0, \] 
\[- I \left( \frac{2\pi \bar{r}_j}{d_j} + k_j \right) \sum_{\mathbf{q} \in \mathbb{Z}^2} \left( \frac{2\pi \bar{q}_k}{d_k} + k_k \right) K^{\bar{r}_1 - \bar{q}_1} r_2 - \bar{q}_2 \bar{q}_1 \bar{q}_2 + \omega^2 \sum_{\mathbf{q} \in \mathbb{Z}^2} \rho^{\bar{r}_1 - \bar{q}_1} r_2 - \bar{q}_2 \bar{q}_1 \bar{q}_2 = 0, \] 
\[- I \omega \sum_{\mathbf{q} \in \mathbb{Z}^2} \psi^{\bar{r}_1 - \bar{q}_1} r_2 - \bar{q}_2 \bar{q}_1 \bar{q}_2 - I \omega \sum_{\mathbf{q} \in \mathbb{Z}^2} p^{\bar{r}_1 - \bar{q}_1} r_2 - \bar{q}_2 \bar{q}_1 \bar{q}_2 = 0, \] 
\[- I \omega \sum_{\mathbf{q} \in \mathbb{Z}^2} \psi^{\bar{r}_1 - \bar{q}_1} r_2 - \bar{q}_2 \bar{q}_1 \bar{q}_2 - I \omega \sum_{\mathbf{q} \in \mathbb{Z}^2} c^{\bar{r}_1 - \bar{q}_1} r_2 - \bar{q}_2 \bar{q}_1 \bar{q}_2 = 0, \] 

where \( k_j \) is the \( j \)th component of the wave vector \( \mathbf{k} \in \mathbb{R}^2 \) and \( \omega = \omega_0 + I \omega_1 \) is the complex angular frequency, whose real and imaginary parts characterize the propagation and the attenuation modes of dispersive Bloch waves, respectively.

Equations (61)–(63) can be expressed in compact form, by introducing the linear operators \( \mathbf{A}, \mathbf{B} \) and \( \mathbf{C} \) applied to the vector \( \mathbf{z} \) that collects the Fourier coefficients of the Bloch amplitudes of \( \bar{\mathbf{u}}_1, \bar{\mathbf{u}}_2, \bar{\mathbf{v}} \) and \( \bar{\mathbf{v}} \); for the details, see Appendix B. This results in

\[(\omega^2 \mathbf{A} + \omega \mathbf{B} + \mathbf{C}) \mathbf{z} = \mathbf{0}, \] 

taking the form of a quadratic generalized eigenvalue problem, where \( \omega \) and \( \mathbf{z} \) are the generalized eigenvalue and eigenvector, respectively. It is worth noting that \( \mathbf{z} \) is the polarization vector of the damped Bloch wave.

The quadratic generalized eigenvalue problem (64) can be transformed into the following equivalent linear generalized eigenvalue problem:

\[(\omega \mathbf{A}' + \mathbf{B}') \mathbf{z}' = \mathbf{0}', \] 

where \( \mathbf{A}' = \mathbf{A} + \mathbf{I} \mathbf{B} \) and \( \mathbf{B}' = \mathbf{B} + \omega^2 \mathbf{C} \).
where the operators \( A' \) and \( B' \) are applied to the generalized eigenvector \( z' \) collecting the vectors \( \omega z \) and \( z \) appearing in (64), see Appendix B. Note that the linear generalized eigenvalue problem (65) has a non-trivial solution \( z' \) if and only if the linear operator \( B' + \omega A' \) is not invertible. In general, an infinite number of generalized eigenvalues \( \omega \) is obtained.

4 Truncation of the generalized eigenvalue problem and approximate solution of the Floquet–Bloch spectrum

The eigenvalue problem (65) corresponds to the compact form of the infinite-dimensional algebraic system of Eqs. (61)–(63). Therefore, in order to obtain an approximate solution for the generalized eigenvalue \( \omega \), the aforementioned algebraic system is truncated by restricting the discrete variables \( \tilde{r}, \tilde{q} \) to the set \([0, Q, \ldots, Q]^2\), with \( Q \in \mathbb{Z}^+ \). It follows that the resulting finite algebraic linear system is characterized by the same number of equations and unknowns, thus resulting in

\[
- \left( \frac{2\pi \tilde{r}_j}{d_j} + k_j \right) \sum_{\tilde{q} \in \{-Q, \ldots, Q\}^2} \left( \frac{2\pi \tilde{q}_k}{d_k} + k_k \right) C_{ijkh} \tilde{r}_z \tilde{q}_z \tilde{u}_h \tilde{q}_y \\
- I \left( \frac{2\pi \tilde{r}_j}{d_j} + k_j \right) \sum_{\tilde{q} \in \{-Q, \ldots, Q\}^2} \alpha_{ij} \tilde{r}_z \tilde{q}_y \tilde{q}_z \\
- I \left( \frac{2\pi \tilde{r}_j}{d_j} + k_j \right) \sum_{\tilde{q} \in \{-Q, \ldots, Q\}^2} \beta_{ij} \tilde{r}_z \tilde{q}_y \tilde{q}_z + \omega^2 \sum_{\tilde{q} \in \{-Q, \ldots, Q\}^2} \rho \tilde{r}_z \tilde{q}_y \tilde{q}_z \tilde{u}_i = 0, \tag{66}
\]

\[
- \left( \frac{2\pi \tilde{r}_i}{d_i} + k_i \right) \sum_{\tilde{q} \in \{-Q, \ldots, Q\}^2} \left( \frac{2\pi \tilde{q}_j}{d_j} + k_j \right) K_{ij} \tilde{r}_z \tilde{q}_y + \omega \sum_{\tilde{q} \in \{-Q, \ldots, Q\}^2} \psi \tilde{r}_z \tilde{q}_y \tilde{q}_z + 2 \tilde{u}_i = \omega \sum_{\tilde{q} \in \{-Q, \ldots, Q\}^2} \psi \tilde{r}_z \tilde{q}_y \tilde{q}_z = 0, \tag{67}
\]

\[
- \left( \frac{2\pi \tilde{r}_i}{d_i} + k_i \right) \sum_{\tilde{q} \in \{-Q, \ldots, Q\}^2} \left( \frac{2\pi \tilde{q}_j}{d_j} + k_j \right) D_{ij} \tilde{r}_z \tilde{q}_y + \omega \sum_{\tilde{q} \in \{-Q, \ldots, Q\}^2} \psi \tilde{r}_z \tilde{q}_y \tilde{q}_z = 0, \tag{68}
\]

In Eqs. (66)–(68), the indices of the Fourier coefficients \( \tilde{u}_i \tilde{q}_y \tilde{q}_z \), \( \tilde{g}_i \tilde{q}_y \tilde{q}_z \), \( \tilde{n}_i \tilde{q}_y \tilde{q}_z \) result as \( \tilde{q} = (\tilde{q}_1, \tilde{q}_2) \in \{-Q, \ldots, Q\}^2 \). Concerning the Fourier coefficients associated with the components of the constitutive tensors, instead, the related indices are \( \tilde{r} - \tilde{q} = (\tilde{r}_1 - \tilde{q}_1, \tilde{r}_2 - \tilde{q}_2) \in \{-2Q, \ldots, 2Q\}^2 \), since it also results in \( \tilde{r} = (\tilde{r}_1, \tilde{r}_2) \in \{-Q, \ldots, Q\}^2 \). Properly conceived convergence analyses will thus be required as \( Q \), i.e. the number of considered harmonics related to the dimension of the finite-dimensional algebraic system, increases.
It is worth noting that we are interested in the study of multi-phase materials, in which the components of the constitutive tensors are discontinuous. In this context, the undesired Gibbs phenomenon arises when an approximate solution is sought, i.e. when the infinite weighted Dirac combs are replaced by finite weighted Dirac combs. This means that spurious oscillations appear in the inverse Fourier transforms of the finite weighted Dirac combs, in the neighbourhood of the discontinuities between material phases. A regularization technique is, thus, required in order to significantly reduce such oscillations, see [34]. Moreover, by adopting the regularization technique an additional benefit is found. It is, indeed, possible to account for a reduced number of harmonics \( Q \) in order to practically fulfil the convergence.

By way of example, we consider a generic component \( C_{ijhk}(x) \) of the elastic tensor and compute the inverse Fourier transform of the associated infinite weighted Dirac comb, as

\[
C_{ijhk}(x) = \sum_{\tilde{r} \in \mathbb{Z}^2} \tilde{C}_{ijhk} \frac{\tilde{r}_1 \tilde{r}_2}{4\pi^2} e^{i(\tilde{r} \cdot x)}.
\]  

(69)

When the infinite weighted Dirac comb is truncated, we obtain its finite-dimensional approximation, denoted with the superscript \((f)\), as

\[
C_{ijhk}^{(f)}(x) = \sum_{\tilde{r} \in \{-2Q,...,2Q\}^2} \tilde{C}_{ijhk} \frac{\tilde{r}_1 \tilde{r}_2}{4\pi^2} e^{i(\tilde{r} \cdot x)}.
\]  

(70)

Finally, a regularization of the approximation above is obtained, by replacing each Fourier coefficient \( \tilde{C}_{ijhk} \) with

\[
\tilde{C}_{ijhk}^{(reg)} = \tilde{C}_{ijhk} e^{-\sigma(\tilde{r}_1^2 + \tilde{r}_2^2)},
\]  

(71)

where the regularization parameter \( \sigma > 0 \) is introduced, involved in the decaying exponential factor \( e^{-\sigma(\tilde{r}_1^2 + \tilde{r}_2^2)} \). After introducing the regularization, Eq. (70) becomes

\[
C_{ijhk}^{(f, reg)}(x) = \sum_{\tilde{r} \in \{-2Q,...,2Q\}^2} \tilde{C}_{ijhk}^{(reg)} \frac{\tilde{r}_1 \tilde{r}_2}{4\pi^2} e^{i(\tilde{r} \cdot x)}.
\]  

(72)

In order to achieve a good trade-off between the reduction in the oscillations near the discontinuities, and the accuracy of the approximation in the periodic cell \( A \), the value of the parameter \( \sigma \) is chosen depending on the considered number of terms in the truncated Fourier expansion.

The effectiveness of such a regularization is demonstrated in Fig. 2 where the component \( C_{1111} \), related to a specific periodic cell with geometry in Fig. 1b, is shown. In Fig. 2a the dimensionless component \( C_{1111}^{(f)}/C^{(ref)} \) and in Fig. 2b the dimensionless component \( C_{1111}^{(f, reg)}/C^{(ref)} \) (where \( C^{(ref)} \) is a reference value) are reported versus the dimensionless coordinates \( x_1/d_1, x_2/d_2 \).

**Fig. 2**

(a) Component \( C_{1111}^{(f)}/C^{(ref)} \), with 961 terms kept in the Fourier expansion; (b) component \( C_{1111}^{(f, reg)}/C^{(ref)} \) with \( \sigma = 0.005 \).
The same procedure (69)–(72) analogously applies to $K_{ij}$, $D_{ij}$, $\alpha_{ij}$, $\beta_{ij}$, $\Psi$, $\rho$, $p$, $c$.

It follows that the infinite-dimensional operators $A$, $B$, $C$ are replaced by their finite-dimensional regularized counterparts $A^{(f, \text{reg})}$, $B^{(f, \text{reg})}$, $C^{(f, \text{reg})}$, and the generalized quadratic eigenvalue problem (64) becomes

$$
\left( \omega^2 A^{(f, \text{reg})} + \omega B^{(f, \text{reg})} + C^{(f, \text{reg})} \right) \tilde{z}^{(f, \text{reg})} = 0^{(f)},
$$

(73)

where the vector $\tilde{z}^{(f, \text{reg})}$ collects the Fourier coefficients of the finite-dimensional Bloch amplitudes of $\tilde{u}_1^{(f, \text{reg})}$, $\tilde{u}_2^{(f, \text{reg})}$, $\tilde{\vartheta}^{(f, \text{reg})}$, $\tilde{\eta}^{(f, \text{reg})}$; for the details, see Appendix B. It is worth remarking that, in our specific model, the matrices associated with the operators $A^{(f, \text{reg})}$ and $B^{(f, \text{reg})}$ are singular. As a consequence, also the matrix associated with the operator $A^{(f, \text{reg})}$ is singular. Then, the linear generalized eigenvalue problem (74) cannot be reduced to a classical eigenvalue problem simply by inverting that matrix. So, suitable spectral transformations and numerical methods are needed for finding the generalized eigenvalues or their subset [53, Chapter 9].

The solution $\omega$ of the generalized eigenvalue problem (73) is an approximation, including a finite number of eigenvalues, of the corresponding generalized eigenvalue solution of (64). Note that the dimension of $z^{(f, \text{reg})}$ is $4(2Q + 1)^2$, since $(2Q + 1)^2$ Fourier coefficients are considered for each of the four unknown Bloch amplitudes $\tilde{u}(x)$, $\tilde{\vartheta}(x)$ and $\tilde{\eta}(x)$, having $\tilde{u}(x)$ two components. Consistently to what done in Eq. (65), the linear generalized eigenvalue problem equivalent to (73) is

$$
(\omega A^{(f, \text{reg})} + B^{(f, \text{reg})}) \tilde{z}^{(f, \text{reg})} = 0^{(f)},
$$

(74)

where, in this case, the operators $A^{(f, \text{reg})}$ and $B^{(f, \text{reg})}$ are applied to the generalized eigenvector $\tilde{z}^{(f, \text{reg})}$ collecting the vectors $\omega z^{(f, \text{reg})}$ and $z^{(f, \text{reg})}$ appearing in (73), see Appendix B.

Finally, the generalized eigenvalues $\omega$, i.e. the complex frequencies, associated with the problem (74) are obtained as the roots of the characteristic equation

$$
\det (\omega A^{(f, \text{reg})} + B^{(f, \text{reg})}) = 0.
$$

(75)

Such a characteristic equation, thus, provides the complex frequency band structure of the thermo-diffusive periodic material.

As detailed in Appendix B, $A^{(f, \text{reg})}$, $B^{(f, \text{reg})}$ and $C^{(f, \text{reg})}$, together with $A^{(f, \text{reg})}$ and $B^{(f, \text{reg})}$, that are constructed starting from the former group, are complex operators. Moreover, the operators $B^{(f, \text{reg})}$ and $C^{(f, \text{reg})}$ depend on the wave vector $\mathbf{k}$ linearly and quadratically, respectively, while $A^{(f, \text{reg})}$ is constant with respect to $\mathbf{k}$. This property can be exploited to speed up their construction as $\mathbf{k}$ varies. Due to this dependence on $\mathbf{k}$, also the generalized eigenvalues $\omega$ depend on $\mathbf{k}$.

4.1 Specialization of the generalized eigenvalue problem to the case of orthotropic or isotropic material phases

In the case of periodic thermo-diffusive materials, characterized by orthotropic phases, in which the orthotropic directions are parallel to the reference system, Eqs. (66)–(68) strongly simplify and take the following form, with all the indices made explicit:

- $-\left( \frac{2\pi \bar{r}_1}{d_1} + k_1 \right) \sum_{q \in [-Q, \ldots, Q]^2} \left( \frac{2\pi \bar{q}_1}{d_1} + k_1 \right) C_{1111}^{\bar{r}_1 \bar{q}_1 \bar{r}_2 \bar{q}_2} (\text{reg}) \tilde{u}_1^{(f, \text{reg})}$

- $-\left( \frac{2\pi \bar{r}_1}{d_1} + k_1 \right) \sum_{q \in [-Q, \ldots, Q]^2} \left( \frac{2\pi \bar{q}_2}{d_2} + k_2 \right) C_{1122}^{\bar{r}_1 \bar{q}_1 \bar{r}_2 \bar{q}_2} (\text{reg}) \tilde{u}_2^{(f, \text{reg})}$

- $-\left( \frac{2\pi \bar{r}_2}{d_2} + k_2 \right) \sum_{q \in [-Q, \ldots, Q]^2} \left( \frac{2\pi \bar{q}_1}{d_1} + k_1 \right) C_{1212}^{\bar{r}_1 \bar{q}_1 \bar{r}_2 \bar{q}_2} (\text{reg}) \tilde{u}_2^{(f, \text{reg})}$

- $-\left( \frac{2\pi \bar{r}_2}{d_2} + k_2 \right) \sum_{q \in [-Q, \ldots, Q]^2} \left( \frac{2\pi \bar{q}_2}{d_2} + k_2 \right) C_{1212}^{\bar{r}_1 \bar{q}_1 \bar{r}_2 \bar{q}_2} (\text{reg}) \tilde{u}_2^{(f, \text{reg})}$
\[-I \left( \frac{2\pi \tilde{r}_1}{d_1} + k_1 \right) \sum_{\tilde{q} \in \{-Q,...,Q\}^2} \tilde{r}_{11} \tilde{q}_1 \tilde{r}_{22} \tilde{q}_2 \left( \text{reg} \right) \tilde{\alpha}_{11} \tilde{q}_1 \tilde{q}_2 \left( \text{reg} \right) \]

\[-I \left( \frac{2\pi r_1}{d_1} + k_1 \right) \sum_{\tilde{q} \in \{-Q,...,Q\}^2} \tilde{r}_{11} \tilde{q}_1 \tilde{r}_{22} \tilde{q}_2 \left( \text{reg} \right) \tilde{D}_{11} \tilde{q}_1 \tilde{q}_2 \left( \text{reg} \right) \]

\[\omega^2 \sum_{\tilde{q} \in \{-Q,...,Q\}^2} \tilde{\rho}_{11} \tilde{q}_1 \tilde{r}_{22} \tilde{q}_2 \left( \text{reg} \right) \tilde{u}_1 \tilde{q}_1 \tilde{q}_2 \left( \text{reg} \right) = 0, \quad (76)\]

\[-I \left( \frac{2\pi \tilde{r}_1}{d_1} + k_1 \right) \sum_{\tilde{q} \in \{-Q,...,Q\}^2} \left( \frac{2\pi \tilde{q}_2}{d_2} + k_2 \right) \tilde{r}_{11} \tilde{q}_1 \tilde{r}_{22} \tilde{q}_2 \left( \text{reg} \right) \tilde{C}_{1212} \tilde{u}_1 \tilde{q}_1 \tilde{q}_2 \left( \text{reg} \right) \]

\[-I \left( \frac{2\pi \tilde{r}_1}{d_1} + k_1 \right) \sum_{\tilde{q} \in \{-Q,...,Q\}^2} \left( \frac{2\pi \tilde{q}_1}{d_1} + k_1 \right) \tilde{r}_{11} \tilde{q}_1 \tilde{r}_{22} \tilde{q}_2 \left( \text{reg} \right) \tilde{D}_{1212} \tilde{u}_1 \tilde{q}_1 \tilde{q}_2 \left( \text{reg} \right) \]

\[\omega^2 \sum_{\tilde{q} \in \{-Q,...,Q\}^2} \tilde{\rho}_{11} \tilde{q}_1 \tilde{r}_{22} \tilde{q}_2 \left( \text{reg} \right) \tilde{u}_1 \tilde{q}_1 \tilde{q}_2 \left( \text{reg} \right) = 0, \quad (77)\]

\[-I \left( \frac{2\pi \tilde{r}_1}{d_1} + k_1 \right) \sum_{\tilde{q} \in \{-Q,...,Q\}^2} \left( \frac{2\pi \tilde{q}_1}{d_1} + k_1 \right) \tilde{r}_{12} \tilde{q}_1 \tilde{r}_{22} \tilde{q}_2 \left( \text{reg} \right) \tilde{C}_{1122} \tilde{u}_1 \tilde{q}_1 \tilde{q}_2 \left( \text{reg} \right) \]

\[-I \left( \frac{2\pi \tilde{r}_2}{d_2} + k_2 \right) \sum_{\tilde{q} \in \{-Q,...,Q\}^2} \left( \frac{2\pi \tilde{q}_1}{d_1} + k_1 \right) \tilde{r}_{12} \tilde{q}_1 \tilde{r}_{22} \tilde{q}_2 \left( \text{reg} \right) \tilde{D}_{1122} \tilde{u}_1 \tilde{q}_1 \tilde{q}_2 \left( \text{reg} \right) \]

\[\omega^2 \sum_{\tilde{q} \in \{-Q,...,Q\}^2} \tilde{\rho}_{12} \tilde{q}_1 \tilde{r}_{22} \tilde{q}_2 \left( \text{reg} \right) \tilde{u}_1 \tilde{q}_1 \tilde{q}_2 \left( \text{reg} \right) = 0, \quad (78)\]
It stands to reason that the operators $A^{(f,\text{reg})}$, $B^{(f,\text{reg})}$, $C^{(f,\text{reg})}$, and $A^{(\ell,\text{reg})}$, $B^{(\ell,\text{reg})}$, explicitly defined in Appendix B, are simplified accordingly.

Finally, in the case of isotropic phases the non-vanishing components of the constitutive and coupling tensors become $C_{1111} = C_{2222} = \tilde{E}/(1 - \tilde{\nu}^2)$, $C_{1122} = \tilde{\nu}\tilde{E}/(1 - \tilde{\nu}^2)$, $C_{1212} = \tilde{E}/2(1 + \tilde{\nu})$, $K_{11} = K_{22} = K$, $D_{11} = D_{22} = D$, $\alpha_{11} = \alpha_{22} = \tilde{\alpha}(1 - 2\tilde{\nu})/(1 - \tilde{\nu})$, $\beta_{11} = \beta_{22} = \tilde{\beta}(1 - 2\tilde{\nu})/(1 - \tilde{\nu})$. In particular, in the case of plane state characterized by sym$((\nabla u) e_3 = 0$, $\nabla \theta \cdot e_3 = 0$, $\nabla \eta \cdot e_3 = 0$, with $e_3 = e_1 \times e_2$ being the out-of-plane unit vector, the constants are $\tilde{E} = E/(1 - \tilde{\nu}^2)$, $\tilde{\nu} = \nu/(1 - \nu)$, $\tilde{\alpha} = (1 - 2\nu)/(1 - 3\nu)\alpha$, $\tilde{\beta} = (1 - 2\nu)/(1 - 3\nu)\beta$, while, in the case with $\sigma e_3 = 0$, $q \cdot e_3 = 0$, $j \cdot e_3 = 0$, the constants are $\tilde{E} = E$, $\tilde{\nu} = \nu$, $\tilde{\alpha} = \alpha$, $\tilde{\beta} = \beta$. In all the previous definitions, $E$ is the Young’s modulus, $\nu$ is the Poisson’s ratio, $\alpha$ is the thermal dilatation constant, and $\beta$ is the dissipative expansion constant.

5 Damped wave propagation in SOFC-like devices

The procedure discussed in Sects. 3 and 4, proposed to determine the band structure of thermo-diffusive heterogeneous materials with periodic microstructure, is here specialized to the case of a thermo-elastic periodic material. The focus is, thus, on the thermo-mechanical coupling phenomena, and the ion diffusion is neglected for the sake of simplicity and without loss of generality.

In this context, we consider a periodic multi-phase laminate, generated by the spatial repetition of solid oxide fuel cells (SOFC-like material). In Fig. 3a, generic cell is reported, characterized by dimensions $d_1 = 100 \mu m$, and $d_2 = 440 \mu m$. We assume all the constituents being linear isotropic, perfectly bonded and in plane state characterized by sym$((\nabla u) e_3 = 0$, $\nabla \theta \cdot e_3 = 0$, $\nabla \eta \cdot e_3 = 0$. The phase 1 identifies the ceramic electrolyte of the SOFC cell, and it is made of yttria-stabilized zirconia (YSZ), with Young’s modulus $E = 155 \times 10^9 \text{ N/m}^2$, Poisson ratio $\nu = 0.3$, the heat conduction constant $K = 0.009 \text{ W/(m K)}$, the thermal dilatation constant $\alpha = 4223.75 \times 10^{-6} \text{ N/(m K)}$, inertial terms $\rho = 5.532 \times 10^3 \text{ kg/m}^3$ and $p = 7548.35 \text{ N/(m}^2 \text{ K})$. The phase 2, instead, represents both cathode and anode electrodes, and it is made of nickel oxide (NiO), characterized by $E = 50 \times 10^9 \text{ N/m}^2$, Poisson ratio $\nu = 0.25$, the heat conduction constant $K = 0.034 \text{ W/(m K)}$, the thermal dilatation constant $\alpha = 1250 \times 10^{-3} \text{ N/(m}^2 \text{ K)}$, inertial terms $\rho = 6.67 \times 10^3 \text{ kg/m}^3$ and $p = 10011.26 \text{ N/(m}^2 \text{ K})$. Finally, the phase 3 mimics conductive interconnections, able to connect adjacent SOFC cells, is made of steel with $E = 2.01 \times 10^{11} \text{ N/m}^2$, Poisson ratio $\nu = 0.3$, the heat conduction constant $K = 0.1228 \text{ W/(m K)}$, the thermal dilatation constant $\alpha = 6030 \times 10^{-3} \text{ N/(m}^2 \text{ K)}$, inertial terms $\rho = 7.86 \times 10^3 \text{ kg/m}^3$ and $p = 13459.7 \text{ N/(m}^2 \text{ K})$.

A set of numerical applications is herein reported, aimed at investigating the complex band structure of the periodic material, as the direction of wave propagation varies. In particular, we analyse both the cases with and without thermo-mechanical coupling (the thermal dilatation tensor $\alpha$ is either different or equal to zero, respectively), in order to grasp the role of the coupling phenomena on the overall material behaviour. We consider three unit vectors of propagation in the first Brillouin zone $m_i \in B$, the first $m_1 = e_1$ propagating parallel to the material layers, the second $m_2 = e_2$ propagating orthogonal to the material layers, while the third $m_3 = d_3/\sqrt{d_1^2 + d_2^2 + d_3^2} + d_1/\sqrt{d_1^2 + d_3^2} e_2$. For the sake of convenience, let us define the dimensionless wave vector $k^* = k_1^* e_1 + k_2^* e_2 \in B^*$, being $k_1^* = k_1 d_1$ and $k_2^* = k_2 d_2$ the dimensionless wave numbers, and the dimensionless first Brillouin zone $B^* = [-\pi, \pi] \times [-\pi, \pi]$. It is, consequently, possible to define the unit vector of propagation $m^* = k^*/||k^*||$. The three considered unit vectors of propagation, thus, become $m_1^* = e_1$, $m_2^* = e_2$ and $m_3^* = \sqrt{2}/2 e_1 + \sqrt{2}/2 e_2$. 
It stands to reason that, under the working hypothesis of thermo-mechanical coupling, the algebraic linear system generated by Eqs. (66)–(68) assumes a reduced form, in which only the equations of the form (66) and (67) are taken into account. Moreover, it results in that the terms containing $\bar{\beta} r_1 - \bar{q}_1$, $\bar{r}_2 - \bar{q}_2$ and $\bar{\eta} q_1 - \bar{q}_2$ are neglected, and the unknowns are reduced to $\tilde{u}_1 q_2$, $\tilde{u}_2 q_2$ and $\tilde{\psi} q_1 q_2$. As a consequence, the equations in compact form (73) and (74) still apply, provided that reduced dimensions of the vectors $z^{(f, \text{reg})}$, $z^{(f, \text{reg})}$ and of the operators $A^{(f, \text{reg})}$, $B^{(f, \text{reg})}$, $C^{(f, \text{reg})}$, $A^{(f, \text{reg})}$, $B^{(f, \text{reg})}$ are considered. Note that the numerical simulations have been repeated for different values of $Q$, in order to test the convergence of the results as the number of considered harmonics increases.

The equivalent linear generalized eigenvalue problem in Eq. (74) has been solved using MATLAB® together with the Advanpix Multiprecision Computing Toolbox, which enables the use of higher precision with respect to the standard double precision, up to quad precision. Such advanced computational tool is here required because, in the specific settings investigated in the numerical simulations, typically the components of the matrices associated with the operators $A^{(f, \text{reg})}$ and $B^{(f, \text{reg})}$, related either to the mechanical, to the thermal or to the coupling parts, are characterized by different orders of magnitude between each other. Moreover, in order to compute the generalized eigenvalues, since the matrices associated with the operators $A^{(f, \text{reg})}$ and $B^{(f, \text{reg})}$ are in general neither symmetric, nor Hermitian, their preliminary generalized Schur decomposition has been exploited [30]. In addition, in order to reduce as much as possible the computational noise and improve the accuracy, a preconditioning of such matrices has been performed, by exploiting the algorithm developed in [63]. More precisely, this preconditioning replaces the operators $A^{(f, \text{reg})}$ and $B^{(f, \text{reg})}$, respectively, with $T_1 A^{(f, \text{reg})} T_2$ and $T_1 B^{(f, \text{reg})} T_2$, where $T_1$ and $T_2$ are suitable invertible operators, determined in accordance with [63]. The joint use of multi-precision and preconditioning is also justified by the fact that, typically, by varying the wave vector $k$, in the specific settings investigated in the numerical simulations, the matrices associated with the operators $A^{(f, \text{reg})}$ and $B^{(f, \text{reg})}$ are characterized by entries with largest absolute value which differ by several orders of magnitude. Finally, for the optimization of the numerical code, a sparse representation of the aforementioned matrices has been adopted, together with their suitable reorganization according to a block structure.
5.1 Numerical examples

In the case with thermo-mechanical coupling, considering the first unit vector of propagation $\mathbf{m}_1^*$, in Fig. 4 the regularized dispersive curves for $Q = 4$, adopting a regular discretization of the variable $k_1$ with 500 points, are shown. In particular, Fig. 4a reports the complex spectrum where both the dimensionless real part $\omega^*_R = \omega_R/\omega_{\text{ref}}$, with $\omega_{\text{ref}} = 1$ rad/s, and imaginary part $\omega^*_I = \omega_I/\omega_{\text{ref}}$ of the complex angular frequency are plotted against the dimensionless wave number $k_1^*$. A high spectral density is observed in the low-frequency range, characterized by both acoustic and gathered optical branches. Temporal damping modes are detected in the plane $\omega^*_R = 0$, while for $\omega^*_R > 0$ mixed modes appear, characterized in general by non-vanishing values of both $\omega^*_R$ and $\omega^*_I$. It is, however, noted that as $\omega^*_R$ decreases the mixed modes tend towards propagation modes since $\omega^*_I$ vanishes. In Fig. 4b, a zoomed view of the acoustic and first four optical branches is reported. Moreover, in Fig. 4c the temporal damping modes are shown separately. Several points of crossing between acoustic and optical branches and also veering phenomena, i.e. repulsion between two branches, are evident. Finally, in Fig. 4d a projection view on the plane $\omega^*_R-k_1^*$ is reported, where the high spectral density prevents the presence of partial band gaps associated with waves with unit vector of propagation $\mathbf{m}_1^*$.

It is observed that the imaginary parts of the complex generalized eigenvalues turn out to be always non-negative, i.e. only damped waves are detected in the material. Moreover, the spectrum results to be anti-symmetric with respect both to the plane $\omega^*_R-k_1^*$ and to the plane $\omega^*_R-\omega^*_I$ characterizing the progressive and regressive waves propagating in the periodic medium. By exploiting these symmetry conditions, the only octant with positive values of $k_1^*$, $\omega^*_R$, $\omega^*_I$ is plotted in Figs. 4a, b. Moreover, the real parts of the complex generalized eigenvalues are typically of some orders of magnitude larger than the corresponding imaginary parts, thus confirming the need of a very high precision enabled by the Advanpix Multiprecision Computing Toolbox.
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Fig. 5 Complex Floquet–Bloch spectrum of the thermo-elastic SOFC-like material related to waves with unit vector of propagation \( \mathbf{m}_1 \). a Complex frequencies \( \omega = \omega^R + i \omega^I \) versus \( k_2^* \); b zoomed view of the lowest frequency branches of Fig. 5a; c view of the dispersive curves associated with temporal damping modes; d projection view on the plane \( \omega^R - k_2^* \).

Analogously, in Fig. 5 the complex Floquet–Bloch spectrum associated with the unit vector of propagation \( \mathbf{m}_3^* \) is investigated. In particular, in Fig. 5a \( \omega^R \) and \( \omega^I \) are plotted versus the dimensionless wave number \( k_3^* \). Again in Fig. 5b, a zoomed view of the lowest frequency branches of Fig. 5a is shown. Figure 5c illustrates the temporal damping modes in the plane \( \omega^R = 0 \). Finally, in Fig. 5d the projection view on the plane \( \omega^R - k_3^* \) is shown. Two partial band gaps are herein detected in the low-frequency range.

In Fig. 6, finally, the unit vector of propagation \( \mathbf{m}_3^* \) is taken into account. In this case, \( k_3^* \) is the wave number in the direction of \( \mathbf{m}_3^* \). Herein, Fig. 6a shows \( \omega^R \) and \( \omega^I \) versus the dimensionless wave number \( k_3^* \), while in Fig. 6b a zoomed view of the lowest frequency branches is reported. In Fig. 6c, various crossing points, together with two veering points, are evident in the temporal damping modes. Due to the high spectral density, no partial band gaps are detected in the projection view on the plane \( \omega^R - k_3^* \), as shown in Fig. 6d.

A final investigation concerns the comparison of Floquet–Bloch spectra in the cases with and without thermo-mechanical coupling, depending on whether the components of the tensor \( \alpha \) are non-vanishing or vanishing, respectively. Therefore, in Figs. 7, 8 and 9 the red curves refer to the case with thermo-mechanical coupling, while the blue ones refer to the case without coupling. In particular, it is possible to emphasize that a qualitatively different behaviour is shown in the two considered cases. In the case with coupling, indeed, mixed modes are detected, while when the coupling is neglected only pure propagation modes appear. Moreover, the blue and red curves tend to increasingly depart from each other as \( \omega^R \) increases. In Fig. 7a, the mixed modes (red curves) and the propagation modes (blue curves) in a low-frequency range are shown, considering the unit vector of propagation \( \mathbf{m}_1^* \). In Fig. 7b, a projection view on the plane \( \omega^R - k_1^* \) of the complex spectrum is shown with \( 0 \leq \omega^R \leq 1.5 \times 10^8 \). It stands to reason that while mixed modes are characterized by non-vanishing values of \( \omega^I \), the propagation modes are defined for \( \omega^I = 0 \). Analogous considerations apply when the unit vector of propagation \( \mathbf{m}_2^* \), as shown in Fig. 8, and the unit vector of propagation \( \mathbf{m}_3^* \), as shown in Fig. 9, are considered. In both Figs. 8b and 9b, the projection view is shown with \( 0 \leq \omega^R \leq 1.5 \times 10^8 \).
Fig. 6 Complex Floquet–Bloch spectrum of the thermo-elastic SOFC-like material related to waves with unit vector of propagation $\mathbf{m}_3^*$. a Complex frequencies $\omega = \omega_R^* + i \omega_I^*$ versus $k_3^*$; b zoomed view of the lowest frequency branches of Fig. 4a; c view of the dispersive curves associated with temporal damping modes; d projection view on the plane $\omega_R^* - k_3^*$

Fig. 7 Comparison of the complex Floquet–Bloch spectra, of SOFC-like material, between the cases with thermo-mechanical coupling (red curves) and without coupling (blue curves) with unit vector of propagation $\mathbf{m}_1^*$. a Complex frequencies $\omega = \omega_R^* + i \omega_I^*$ versus $k_1^*$; b projection view on the plane $\omega_R^* - k_1^*$ (colour figure online)

6 Final remarks

Thermo-diffusion phenomena involving SOFC-like periodic materials have been investigated in the dynamic regime. Adopting a micromechanical approach, the dispersive wave propagation within the periodic medium has been analysed taking into account coupling effects between thermal mechanical and diffusive phenomena. To this aim, a generalization of the Floquet–Bloch theory has been adopted in order to determine the complex-
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Fig. 8 Comparison of the complex Floquet–Bloch spectra, of SOFC-like material, between the cases with thermo-mechanical coupling (red curves) and without coupling (blue curves) with unit vector of propagation $m_2^\star$. a Complex frequencies $\omega = \omega_R^\star + I \omega_I^\star$ versus $k_2^\star$; b projection view on the plane $\omega_I^\star - k_2^\star$ (colour figure online)

Fig. 9 Comparison of the complex Floquet–Bloch spectra, of SOFC-like material, between the cases with thermo-mechanical coupling (red curves) and without coupling (blue curves) with unit vector of propagation $m_3^\star$. a Complex frequencies $\omega = \omega_R^\star + I \omega_I^\star$ versus $k_3^\star$; b projection view on the plane $\omega_I^\star - k_3^\star$ (colour figure online)

valued frequency band structure of such materials. The Christoffel equation has been obtained from the governing equations of the first-order thermo-diffusive medium. By adopting the Floquet–Bloch decomposition and exploiting proper integral transforms, an infinite algebraic linear system, involving complex frequencies and wave vectors, has been determined. Such infinite system has been truncated taking into account a limited number of equations, which number has been obtained via a convergence analysis. In order to avoid the well-known Gibbs phenomenon, a regularization technique has been utilized. Finally, the complex angular frequencies, corresponding to a given wave vector, are found by solving the finite sequence of unknowns and eigenvalue problems resulting from a discretization of the wave vector space.

The numerical investigations concern a periodic cell mimicking a SOFC device, in which the diffusive phenomena are neglected. Considering the thermo-mechanical coupling, the complex dispersion curves in the first Brillouin zone, examined in the dimensionless space, are reported for three unit vectors of propagation. In general, a high spectral density is observed in the low-frequency range, characterized both by acoustic and gathered optical branches. Both temporal damping modes and mixed modes feature the band structure of the periodic material. In particular, the mixed modes tend towards propagation modes as the real part of the complex frequency decreases. Concerning the temporal damping modes, several points of crossing between acoustic and optical branches and also veering phenomena are found. Partial band gaps only characterize waves propagating orthogonally to the material layers, while no partial band gaps are associated with the other two considered unit vectors of propagation.

Finally, in order to emphasize the effects of coupling phenomena, also the uncoupled problem is investigated. Qualitatively different behaviours are observed. Indeed, it results in that in the absence of coupling
phenomena the mixed modes tend to become propagation modes, and only the real part of the complex frequencies is different from zero.

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Appendix A: Explicit form of the governing equations in the transformed space

By exploiting the convolution products, Eqs. (39)–(41) can be written in the following form:

\[ I r_j \int_{\mathbb{R}^2} \mathcal{F}_x[C_{ijhk}] (q - q) \left( I q_k \int_{\mathbb{R}^2} \mathcal{F}_x[\tilde{u}_h] (q - w) \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) \, dw \right) \, dq \]
\[ - I r_j \int_{\mathbb{R}^2} \mathcal{F}_x[\alpha_{ij}] (r - q) \left( I q_k \int_{\mathbb{R}^2} \mathcal{F}_x[\tilde{\theta}] (q - w) \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) \, dw \right) \, dq \]
\[ - I r_j \int_{\mathbb{R}^2} \mathcal{F}_x[\beta_{ij}] (r - q) \left( I q_k \int_{\mathbb{R}^2} \mathcal{F}_x[\tilde{u}_i] (q - w) \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) \, dw \right) \, dq \]
\[ + \omega^2 \int_{\mathbb{R}^2} \mathcal{F}_x[p] (r - q) \left( I q_j \int_{\mathbb{R}^2} \mathcal{F}_x[\tilde{u}_i] (q - w) \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) \, dw \right) \, dq = 0, \quad (80) \]

\[ I r_i \int_{\mathbb{R}^2} \mathcal{F}_x[K_{ij}] (r - q) \left( I q_j \int_{\mathbb{R}^2} \mathcal{F}_x[\tilde{\theta}] (q - w) \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) \, dw \right) \, dq \]
\[ - I \omega \int_{\mathbb{R}^2} \mathcal{F}_x[\alpha_{ij}] (r - q) \left( I q_j \int_{\mathbb{R}^2} \mathcal{F}_x[\tilde{\theta}] (q - w) \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) \, dw \right) \, dq \]
\[ - I \omega \int_{\mathbb{R}^2} \mathcal{F}_x[\Psi] (r - q) \left( I q_j \int_{\mathbb{R}^2} \mathcal{F}_x[\tilde{u}_i] (q - w) \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) \, dw \right) \, dq \]
\[ - I \omega \int_{\mathbb{R}^2} \mathcal{F}_x[p] (r - q) \left( I q_j \int_{\mathbb{R}^2} \mathcal{F}_x[\tilde{u}_i] (q - w) \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) \, dw \right) \, dq = 0, \quad (81) \]

\[ I r_i \int_{\mathbb{R}^2} \mathcal{F}_x[D_{ij}] (r - q) \left( I q_j \int_{\mathbb{R}^2} \mathcal{F}_x[\tilde{\theta}] (q - w) \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) \, dw \right) \, dq \]
\[ - I \omega \int_{\mathbb{R}^2} \mathcal{F}_x[\beta_{ij}] (r - q) \left( I q_j \int_{\mathbb{R}^2} \mathcal{F}_x[\tilde{u}_i] (q - w) \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) \, dw \right) \, dq \]
\[ - I \omega \int_{\mathbb{R}^2} \mathcal{F}_x[\Psi] (r - q) \left( I q_j \int_{\mathbb{R}^2} \mathcal{F}_x[\tilde{\theta}] (q - w) \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) \, dw \right) \, dq \]
\[ - I \omega \int_{\mathbb{R}^2} \mathcal{F}_x[c] (r - q) \left( I q_j \int_{\mathbb{R}^2} \mathcal{F}_x[\tilde{\theta}] (q - w) \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) \, dw \right) \, dq = 0, \quad (82) \]

with \( r, q, w \in B \). Note that in Eqs. (80), (81), (82) the Fourier transform of the exponential function, i.e. \( \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] \), results in

\[ \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) = 4\pi^2 \delta(w - k), \quad (83) \]

where \( \delta \) is the Dirac-delta generalized function centred at \( w = k \). It follows that the convolution product between the Fourier transform \( \mathcal{F}_x[g(x)] \), with \( g(x) \) a generic function, and \( \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] \) can be written as

\[ \int_{\mathbb{R}^2} \mathcal{F}_x[g(x)] (q - w) \mathcal{F}_x \left[ e^{I \langle k \cdot x \rangle} \right] (w) \, dw \]
\[ = \int_{\mathbb{R}^2} \mathcal{F}_x[g(x)] (q - w) 4\pi^2 \delta(w - k) \, dw = 4\pi^2 \mathcal{F}_x[g(x)] (q - k). \quad (84) \]

Finally, by applying (84) to (80)–(82), one obtains Eqs. (42)–(44).
Appendix B: Linear operators involved in the generalized eigenvalue problems

B.1 Vector \(z\), and operators \(A, B\) and \(C\)

In order to express Eqs. (61)–(63) in compact form, the linear operators \(A, B\) and \(C\) are herein defined, in terms of their actions on the argument \(z\), expressed in the following form:

\[
z = \text{col}(\tilde{u}_1, \tilde{u}_2, \tilde{\vartheta}, \tilde{\eta}) \in (l_2(\mathbb{Z}^2))^4, \tag{85}
\]

where \(\tilde{u}_1, \tilde{u}_2, \tilde{\vartheta}, \tilde{\eta}\) are vectors collecting, respectively, the Fourier coefficients \(\tilde{u}_1^{\tilde{q}_1\tilde{q}_2}, \tilde{u}_2^{\tilde{q}_1\tilde{q}_2}, \tilde{\vartheta}^{\tilde{q}_1\tilde{q}_2}, \tilde{\eta}^{\tilde{q}_1\tilde{q}_2}\), the col operator stacks its vector arguments column-wise into a single column vector, \(l_2(\mathbb{Z}^2)\) denotes the space of square-summable sequences with two integer indices and \((l_2(\mathbb{Z}^2))^4\) stands for \(l_2(\mathbb{Z}^2) \times l_2(\mathbb{Z}^2) \times l_2(\mathbb{Z}^2) \times l_2(\mathbb{Z}^2)\).

The first operator \(A : (l_2(\mathbb{Z}^2))^4 \rightarrow (l_2(\mathbb{Z}^2))^4\) is defined equation-wise as follows:

\[
\begin{align*}
A \text{col}(\tilde{u}_1, \tilde{u}_2, \tilde{\vartheta}, \tilde{\eta}) & \begin{bmatrix} r_1 \cr r_2 \end{bmatrix}^{\tilde{r}_1 \tilde{r}_2} = \sum_{q \in \mathbb{Z}^2} \rho_{\tilde{r}_1-\tilde{q}_1 \tilde{r}_2-\tilde{q}_2}^{\tilde{q}_1 \tilde{q}_2} \tilde{u}_1^{\tilde{q}_1 \tilde{q}_2}, \quad \tag{86} \\
A \text{col}(\tilde{u}_1, \tilde{u}_2, \tilde{\vartheta}, \tilde{\eta}) & \begin{bmatrix} r_1 \cr r_2 \end{bmatrix}^{\tilde{r}_1 \tilde{r}_2} = \sum_{q \in \mathbb{Z}^2} \rho_{\tilde{r}_1-\tilde{q}_1 \tilde{r}_2-\tilde{q}_2}^{\tilde{q}_1 \tilde{q}_2} \tilde{u}_2^{\tilde{q}_1 \tilde{q}_2}, \quad \tag{87} \\
A \text{col}(\tilde{u}_1, \tilde{u}_2, \tilde{\vartheta}, \tilde{\eta}) & \begin{bmatrix} r_1 \cr r_2 \end{bmatrix}^{\tilde{r}_1 \tilde{r}_2} = 0, \quad \tag{88} \\
A \text{col}(\tilde{u}_1, \tilde{u}_2, \tilde{\vartheta}, \tilde{\eta}) & \begin{bmatrix} r_1 \cr r_2 \end{bmatrix}^{\tilde{r}_1 \tilde{r}_2} = 0. \quad \tag{89}
\end{align*}
\]

The second operator \(B : (l_2(\mathbb{Z}^2))^4 \rightarrow (l_2(\mathbb{Z}^2))^4\) is defined equation-wise as follows:

\[
\begin{align*}
B \text{col}(\tilde{u}_1, \tilde{u}_2, \tilde{\vartheta}, \tilde{\eta}) & \begin{bmatrix} r_1 \cr r_2 \end{bmatrix}^{\tilde{r}_1 \tilde{r}_2} = 0, \quad \tag{90} \\
B \text{col}(\tilde{u}_1, \tilde{u}_2, \tilde{\vartheta}, \tilde{\eta}) & \begin{bmatrix} r_1 \cr r_2 \end{bmatrix}^{\tilde{r}_1 \tilde{r}_2} = 0, \quad \tag{91} \\
B \text{col}(\tilde{u}_1, \tilde{u}_2, \tilde{\vartheta}, \tilde{\eta}) & \begin{bmatrix} r_1 \cr r_2 \end{bmatrix}^{\tilde{r}_1 \tilde{r}_2} = \sum_{q \in \mathbb{Z}^2} \left( \frac{2\pi \tilde{q}_j}{d_j} + k_j \right) \alpha_{\tilde{r}_1-\tilde{q}_1 \tilde{r}_2-\tilde{q}_2}^{\tilde{q}_1 \tilde{q}_2} \tilde{u}_1^{\tilde{q}_1 \tilde{q}_2} \tilde{\vartheta}^{\tilde{q}_1 \tilde{q}_2} - I \sum_{q \in \mathbb{Z}^2} \psi_{\tilde{r}_1-\tilde{q}_1 \tilde{r}_2-\tilde{q}_2}^{\tilde{q}_1 \tilde{q}_2} \tilde{\vartheta}^{\tilde{q}_1 \tilde{q}_2}, \quad \tag{92} \\
B \text{col}(\tilde{u}_1, \tilde{u}_2, \tilde{\vartheta}, \tilde{\eta}) & \begin{bmatrix} r_1 \cr r_2 \end{bmatrix}^{\tilde{r}_1 \tilde{r}_2} = \sum_{q \in \mathbb{Z}^2} \left( \frac{2\pi \tilde{q}_j}{d_j} + k_j \right) \beta_{\tilde{r}_1-\tilde{q}_1 \tilde{r}_2-\tilde{q}_2}^{\tilde{q}_1 \tilde{q}_2} \tilde{u}_1^{\tilde{q}_1 \tilde{q}_2} \tilde{\vartheta}^{\tilde{q}_1 \tilde{q}_2} - I \sum_{q \in \mathbb{Z}^2} \psi_{\tilde{r}_1-\tilde{q}_1 \tilde{r}_2-\tilde{q}_2}^{\tilde{q}_1 \tilde{q}_2} \tilde{\vartheta}^{\tilde{q}_1 \tilde{q}_2}, \quad \tag{93}
\end{align*}
\]

The third operator \(C : (l_2(\mathbb{Z}^2))^4 \rightarrow (l_2(\mathbb{Z}^2))^4\) is defined equation-wise as follows:

\[
\begin{align*}
C \text{col}(\tilde{u}_1, \tilde{u}_2, \tilde{\vartheta}, \tilde{\eta}) & \begin{bmatrix} r_1 \cr r_2 \end{bmatrix}^{\tilde{r}_1 \tilde{r}_2} = \left( \frac{2\pi \tilde{r}_j}{d_j} + k_j \right) \sum_{q \in \mathbb{Z}^2} \left( \frac{2\pi \tilde{q}_k}{d_k} + k_k \right) C_{\tilde{r}_1-\tilde{q}_1 \tilde{r}_2-\tilde{q}_2}^{\tilde{q}_1 \tilde{q}_2} \tilde{u}_1^{\tilde{q}_1 \tilde{q}_2} \tilde{\vartheta}^{\tilde{q}_1 \tilde{q}_2} - I \left( \frac{2\pi \tilde{r}_j}{d_j} + k_j \right) \sum_{q \in \mathbb{Z}^2} \alpha_{\tilde{r}_1-\tilde{q}_1 \tilde{r}_2-\tilde{q}_2}^{\tilde{q}_1 \tilde{q}_2} \tilde{\vartheta}^{\tilde{q}_1 \tilde{q}_2}, \quad \tag{94}
\end{align*}
\]
These operators are expressed, alternatively, in terms of the operators $A$. Moreover, the operators $A$ which shows the equivalence between Eqs. (64) and (65).

These operators are defined as follows:

$$B_{\text{col}} = I$$

and

$$B'_{\text{col}} = I$$

denote the zero and identity infinite-dimensional linear operators from $(l_2(\mathbb{Z}^2))^4$ to $(l_2(\mathbb{Z}^2))^4$, respectively.

The first operator

$$A' : (l_2(\mathbb{Z}^2))^4 \times (l_2(\mathbb{Z}^2))^4 \rightarrow (l_2(\mathbb{Z}^2))^4 \times (l_2(\mathbb{Z}^2))^4$$

is defined as follows:

$$A' z = \text{col} \left( A z_1 + 0 z_2, 0 z_1 + I z_2 \right),$$

where $0$ and $I$ denote the zero and identity infinite-dimensional linear operators from $(l_2(\mathbb{Z}^2))^4$ to $(l_2(\mathbb{Z}^2))^4$, respectively.

The second operator

$$B' : (l_2(\mathbb{Z}^2))^4 \times (l_2(\mathbb{Z}^2))^4 \rightarrow (l_2(\mathbb{Z}^2))^4 \times (l_2(\mathbb{Z}^2))^4$$

is defined as follows:

$$B' z = \text{col} \left( B z_1 + C z_2, -I z_1 + 0 z_2 \right).$$

By applying the operators $A'$ and $B'$ to the vector $z'$ defined as

$$z' = \text{col} (z_1, z_2) = \text{col} (\omega z, z),$$

one gets

$$(\omega A' + B') z' = \text{col} (\omega A \omega z + \omega 0 z + B \omega z + C z, \omega 0 \omega z + \omega I z - I \omega z + 0 z)$$

$$= \text{col} \left( (\omega^2 A + \omega B + C) z, 0 \right),$$

which shows the equivalence between Eqs. (64) and (65).
B.3 Vector $z(f, reg)$ and $z'(f, reg)$, and operators $A(f, reg)$, $B(f, reg)$ and $C(f, reg)$

Concerning the finite-dimensional generalized quadratic eigenvalue problem in Eq. (73), the vector $z(f, reg)$ results in

$$z(f, reg) = \text{col}(u_1(f, reg), u_2(f, reg), \tilde{\theta}(f, reg), \tilde{\eta}(f, reg)) \in (\mathbb{R}^{2(2Q+1)})^4,$$

(105)

where $(\mathbb{R}^{2(2Q+1)})^4$ stands for $\mathbb{R}^{(2Q+1)^2} \times \mathbb{R}^{(2Q+1)^2} \times \mathbb{R}^{(2Q+1)^2} \times \mathbb{R}^{(2Q+1)^2}$.

The operators $A(f, reg)$, $B(f, reg)$, $C(f, reg)$ : $(\mathbb{R}^{2(2Q+1)^2})^4 \rightarrow (\mathbb{R}^{2(2Q+1)^2})^4$ are defined in a similar way as $A$, $B$, and $C$, by restricting $\tilde{\mathbf{r}}$ and $\tilde{\mathbf{q}}$ to $\{-Q, \ldots, Q\}^2$.

Analogously to the infinite-dimensional case, the operators $A'(f, reg)$ and $B'(f, reg)$ in Eq. (74) can be defined, after introducing the argument

$$z'(f, reg) = \text{col}\left(\omega z(f, reg), z'(f, reg)\right) \in (\mathbb{R}^{2(2Q+1)^2})^4 \times (\mathbb{R}^{2(2Q+1)^2})^4.$$

(106)

The first operator $A'(f, reg)$ : $(\mathbb{R}^{2(2Q+1)^2})^4 \times (\mathbb{R}^{2(2Q+1)^2})^4 \rightarrow (\mathbb{R}^{2(2Q+1)^2})^4 \times (\mathbb{R}^{2(2Q+1)^2})^4$ is defined equation-wise as follows:

$$A'(f, reg) z'(f, reg) = \text{col}\left(A(f, reg) \omega z(f, reg) + \theta(f) z'(f, reg), \theta(f) \omega z'(f, reg) + I(f) z'(f, reg)\right),$$

(107)

where $\theta(f)$ and $I(f)$ denote the zero and identity operators from $(\mathbb{R}^{2(2Q+1)^2})^4$ to $(\mathbb{R}^{2(2Q+1)^2})^4$, respectively.

The second operator $B'(f, reg)$ : $(\mathbb{R}^{2(2Q+1)^2})^4 \times (\mathbb{R}^{2(2Q+1)^2})^4 \rightarrow (\mathbb{R}^{2(2Q+1)^2})^4 \times (\mathbb{R}^{2(2Q+1)^2})^4$ is defined equation-wise as follows:

$$B'(f, reg) z'(f, reg) = \text{col}\left(B'(f, reg) \omega z(f, reg) + C(f, reg) z'(f, reg), -I'(f) \omega z'(f, reg) + \theta'(f) \omega z'(f, reg)\right).$$

(108)

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