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On the quasistatic effective elastic moduli for elastic waves in three-dimensional phononic crystals

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Abstract

Effective elastic moduli for 3D solid-solid phononic crystals of arbitrary anisotropy and oblique lattice structure are formulated analytically using the plane-wave expansion (PWE) method and the recently proposed monodromy-matrix (MM) method. The latter approach employs Fourier series in two dimensions with direct numerical integration along the third direction. As a result, the MM method converges much quicker to the exact moduli in comparison with the PWE as the number of Fourier coefficients increases. The MM method yields a more explicit formula than previous results, enabling a closed-form upper bound on the effective Christoffel tensor. The MM approach significantly improves the efficiency and accuracy of evaluating effective wave speeds for high-contrast composites and for configurations of closely spaced inclusions, as demonstrated by three-dimensional examples.

1. Introduction

Long-wave low-frequency dispersion of acoustic waves in periodic structures is of both fundamental and practical interest, particularly due to the current advances in manufacturing of metamaterials and phononic crystals. In this light, the leading order dispersion (quasistatic limit) has recently been under intensive study by various theoretical approaches such as plane-wave expansion (PWE) [1, 2, 3], scaling technique [4, 5], asymptotics of multiple-scattering theory [6, 7, 8] and a newly proposed monodromy-matrix (MM) method [9]. The cases treated were mostly confined to scalar waves in 2D (two-dimensional) structures. Regarding vector waves in 2D and especially in 3D phononic crystals, a variety of methods have been proposed for calculating the quasistatic effective elastic properties of 3D periodic composites containing spherical inclusions arranged in a simple cubic array. For the case of rigid inclusions an integral equation on the sphere surface was solved numerically to obtain the effective properties [10]. Spherical voids [11] and subsequently elastic inclusions were considered using a Fourier series approach [12]. Alternative procedures for elastic spherical inclusions include the method of singular distributions [13] and infinite series of periodic multipole solutions of the equilibrium equations [14]. The latter multipole expansion method has also been applied to cubic arrays of ellipsoidal inclusions [15]. A particular PWE-based method of calculation of quasistatic speeds in 3D phononic crystals of cubic symmetry has been formulated and implemented in [16]. A review of numerical methods for calculating effective properties of composites can be found in [17, §2.8,§14.11].

Of all the methods available for calculating effective elastic moduli the PWE method is arguably the simplest and most straightforward to implement. It requires only Fourier coefficients of the inclusion in the unit cell, which makes it the method of choice for many problems. Unfortunately, PWE is not a very

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practical tool for the 3D case, where the vectors and matrices in the Fourier space are of very large algebraic dimension, especially if the phononic crystal is composed of highly contrasting materials (examples in §5 illustrate this critical drawback).

The present paper provides the PWE and MM analytical formulations of the 21 components of the effective elastic stiffness for 3D solid-solid phononic crystals of arbitrary anisotropy and arbitrary oblique lattice. While the PWE method is widely used in some fields its formulation for general anisotropic static elasticity has, surprisingly, not been discussed before. The PWE is presented here in a compact form (see Eq. (15)) suitable for numerical implementation. The main thrust of the paper is concerned with the MM approach. The motivation for advocating this method as an alternative to the more conventional PWE technique is, first, that the MM method 'spares' Fourier expansion in one of the coordinates (this is particularly advantageous for the 3D numerics) and, second, that the MM method has much faster convergence than PWE. Comparison of the MM and PWE calculations provided in the paper confirms a markedly better efficiency of the MM method.

The paper is organised as follows. In Section 2, the quasistatic perturbation theory is used to define the effective Christoffel equation in the form which serves as the common starting point for the PWE and MM methods. The PWE formulation of the effective elastic moduli follows readily and is also presented in Section 2. The MM formulation is described in Section 3: the derivation of the MM formula is in §3.1 (see also Appendix 1), its numerical implementation is discussed in §3.2, generalization to the case of an oblique lattice is presented in §3.3 and the scheme for recovering the full set of effective elastic moduli is provided in §3.4. A closed-form estimate of the effective Christoffel matrix is presented in Section 4. Examples of the MM and PWE calculations are provided in Section 5. Concluding remarks are given in Section 6.

2. Background. PWE formula

Consider a 3D anisotropic medium with density and elastic stiffness

$$\rho(\mathbf{x}) = \rho(\mathbf{x} + \mathbf{e}_p), \;\; \mathbf{C}(\mathbf{x}) = \mathbf{C}(\mathbf{x} + \mathbf{e}_p), \tag{1}$$

which are assumed to be **1**-periodic, i.e. invariant to period or translation vectors $\mathbf{e}_p = (\delta_{pq})$ (a cubic lattice, otherwise see §3.3). All roman indices run from 1 to 3. In the following, * and $^+$ mean complex and Hermitian conjugation. Assume no dissipation so that the elements of $\mathbf{C}$ satisfy $c_{ijkl} = c^*_{klij}$ ($= c_{klij}$ for real case). Our goal is the quasistatic effective elastic stiffness $\mathbf{C}^{\text{eff}}$ with elements c^{eff}_{ijkl} that have the same symmetries as those of $\mathbf{C}$, and matrices $\mathbf{C}^{\text{eff}}_{jl}$ defined by analogy with Eq. (2). For compact writing, introduce the matrices

$$\mathbf{C}_{jl} = (c_{ijkl})^3_{i,k=1} = \mathbf{C}^+_{lj} \tag{2}$$

with components numbered by i, k. The elastodynamic equation for time-harmonic waves $\mathbf{v}\,(\mathbf{x}, t) = \mathbf{v}(\mathbf{x})e^{-i\omega t}$ is

$$\partial_j(\mathbf{C}_{jl}\partial_l\mathbf{v}) = -\rho\omega^2\mathbf{v}, \tag{3}$$

where $\partial_j \equiv \partial/\partial x_j$ and repeated indices are summed. The differential operator in Eq. (3) is self-adjoint with respect to the Floquet condition $\mathbf{v}(\mathbf{x}) = \mathbf{u}(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}}$ with **1**-periodic $\mathbf{u}(\mathbf{x}) = \mathbf{u}(\mathbf{x} + \mathbf{e}_p)$ and $\mathbf{k} = k\boldsymbol{\kappa}$ ($|\boldsymbol{\kappa}| = 1$). Substituting this condition in (3) casts it into the form

$$\begin{gathered}(\mathcal{C}_0 + k\mathcal{C}_1 + k^2\mathcal{C}_2)\mathbf{u} = \rho\omega^2\mathbf{u}, \quad \text{where} \\ \mathcal{C}_0\mathbf{u} \equiv -\partial_j(\mathbf{C}_{jl}\partial_l\mathbf{u}),\, \mathcal{C}_1\mathbf{u} \equiv -i(\kappa_j\mathbf{C}_{jl}\partial_l + \kappa_l\partial_j\mathbf{C}_{jl})\mathbf{u},\; \mathcal{C}_2\mathbf{u} \equiv \kappa_j\kappa_l\mathbf{C}_{jl}\mathbf{u}.\end{gathered} \tag{4}$$

All operators $\mathcal{C}$ are self-adjoint. We introduce for future use linear, areal and volumetric averages over the unit-cell: $\langle\cdot\rangle_j$ is the average over coordinate x_j; $\langle\cdot\rangle_{\overline{j}}$ is the average over the section orthogonal to x_j, and $\langle\cdot\rangle$ is the complete average. These averages in turn define inner products of vector-valued functions. Thus, for a scalar function f and vector-functions $\mathbf{f}$, $\mathbf{h}$,

$$\langle f\rangle_j = \int_0^1 f dx_j, \quad \langle f\rangle = \int_{[0,1]^3} f d\mathbf{x}, \quad (\mathbf{f},\mathbf{h})_{\overline{j}} = \langle\mathbf{h}^+\mathbf{f}\rangle_{\overline{j}}, \;\; (\mathbf{f},\mathbf{h}) = \langle\mathbf{h}^+\mathbf{f}\rangle. \tag{5}$$

Next we apply perturbation theory to (4) with a view to defining the quasistatic effective Christoffel matrix whose eigenvalues yield the effective speeds

$$c_\alpha \equiv c_\alpha(\boldsymbol{\kappa}) \equiv \lim_{k\to 0} \omega_\alpha(\mathbf{k})/k, \ \ \alpha = 1,2,3. \tag{6}$$

For $k = 0$, the eigenvalue $\omega = 0$ has multiplicity 3 and corresponds to three constant linear independent eigenvectors $\mathbf{u}_{0\alpha}$. Consider the asymptotics

$$\omega_\alpha^2 = 0 + k\lambda_{1\alpha} + k^2\lambda_{2\alpha} + O(k^3), \tag{7a}$$

$$\mathbf{u}_\alpha = \mathbf{u}_{0\alpha} + k\mathbf{u}_{1\alpha} + k^2\mathbf{u}_{2\alpha} + \mathbf{O}(k^3). \tag{7b}$$

Substituting (7) into (4) and collecting terms with the same power of k yields

$$1: \qquad \mathcal{C}_0\mathbf{u}_{0\alpha} = \mathbf{0}, \tag{8a}$$

$$k: \qquad \mathcal{C}_1\mathbf{u}_{0\alpha} + \mathcal{C}_0\mathbf{u}_{1\alpha} = \rho\lambda_{1\alpha}\mathbf{u}_{0\alpha}, \tag{8b}$$

$$k^2: \qquad \mathcal{C}_2\mathbf{u}_{0\alpha} + \mathcal{C}_1\mathbf{u}_{1\alpha} + \mathcal{C}_0\mathbf{u}_{2\alpha} = \rho\lambda_{1\alpha}\mathbf{u}_{1\alpha} + \rho\lambda_{2\alpha}\mathbf{u}_{0\alpha}. \tag{8c}$$

Scalar multiplying (8b) by $\mathbf{u}_{0\alpha}$ and (8c) by $\mathbf{e}_k$, and using $(\mathcal{C}_1\mathbf{u}_{0\alpha}, \mathbf{u}_{0\alpha}) = 0$ together with self-adjointness of $\mathcal{C}_0$ leads to

$$\lambda_{1\alpha} = 0; \ \ \mathbf{u}_{1\alpha} = -\mathcal{C}_0^{-1}\mathcal{C}_1\mathbf{u}_{0\alpha}; \ \ (\mathcal{C}_2\mathbf{u}_{0\alpha}, \mathbf{e}_k) + (\mathcal{C}_1\mathbf{u}_{1\alpha}, \mathbf{e}_k) = \langle\rho\rangle\lambda_{2\alpha}(\mathbf{u}_{0\alpha}, \mathbf{e}_k), \ k = 1,2,3, \tag{9}$$

where $\lambda_{2\alpha} = c_\alpha^2$ due to $\lambda_{1\alpha} = 0$ and (6). Inserting $\mathbf{u}_{1\alpha}$ from $(9)_2$ in $(9)_3$ gives

$$\boldsymbol{\Gamma}\mathbf{u}_{0\alpha} = \langle\rho\rangle c_\alpha^2\mathbf{u}_{0\alpha}, \ \ \alpha = 1,2,3, \tag{10}$$

where $\boldsymbol{\Gamma} = ((\mathcal{C}_2\mathbf{e}_k, \mathbf{e}_i) - (\mathcal{C}_0^{-1}\mathcal{C}_1\mathbf{e}_k, \mathcal{C}_1\mathbf{e}_i))_{i,k=1}^3$. Substituting $\mathcal{C}_1$, $\mathcal{C}_2$ from (4) defines the quasistatic effective 3×3 Christoffel matrix $\boldsymbol{\Gamma} = (\Gamma_{ik})_{i,k=1}^3$ in the form

$$\boldsymbol{\Gamma}(\kappa) = \mathbf{C}_{jl}^{\mathrm{e}}\kappa_j\kappa_l \ \ \text{where} \ \ \mathbf{C}_{jl}^{\mathrm{e}} \equiv \langle\mathbf{C}_{jl}\rangle - \langle(\partial_p\mathbf{C}_{pj}^+)\mathcal{C}_0^{-1}(\partial_q\mathbf{C}_{ql})\rangle \ \big(= \mathbf{C}_{lj}^{\mathrm{e}+}\big). \tag{11}$$

The matrix $\mathbf{C}_{jl}^{\mathrm{e}}$ is distinguished from $\mathbf{C}_{jl}^{\mathrm{eff}}$, in terms of which the Christoffel matrix is

$$\boldsymbol{\Gamma}(\kappa) = \mathbf{C}_{jl}^{\mathrm{eff}}\kappa_j\kappa_l = \frac{1}{2}\big(\mathbf{C}_{jl}^{\mathrm{eff}} + \mathbf{C}_{lj}^{\mathrm{eff}}\big)\kappa_j\kappa_l. \tag{12}$$

Comparison of Eqs. $(11)_1$ and (12) implies that $\mathbf{C}_{jl}^{\mathrm{e}}$ and $\mathbf{C}_{jl}^{\mathrm{eff}}$ are related by

$$\mathbf{C}_{jl}^{\mathrm{eff}} + \mathbf{C}_{lj}^{\mathrm{eff}} = \mathbf{C}_{jl}^{\mathrm{e}} + \mathbf{C}_{lj}^{\mathrm{e}} \tag{13}$$

and they are equal if $j = l$. Equation $(11)_2$ does not yield $\mathbf{C}_{jl}^{\mathrm{eff}}$ explicitly, only in the combination (13); however, this connection is sufficient for the purpose of finding all elements of $\mathbf{C}^{\mathrm{eff}}$, as described in §3.4. For now we focus on methods to calculate $\mathbf{C}_{jl}^{\mathrm{e}}$.

Equation $(11)_2$ is still an implicit formula for the matrix $\mathbf{C}_{jl}^{\mathrm{e}}$ in so far as the operator $\mathcal{C}_0^{-1}$ is not specified. One way to an explicit implementation of $(11)_2$ is via its transformation to Fourier space which must be truncated to define $\mathcal{C}_0^{-1}$ as a matrix inverse. Thus taking the 3D Fourier expansion

$$\mathbf{C}_{jl}(\mathbf{x}) = \sum\nolimits_{\mathbf{g}\in\mathbb{Z}^3}\widehat{\mathbf{C}}_{jl}(\mathbf{g})e^{2\pi i\mathbf{g}\cdot\mathbf{x}}, \ \ \widehat{\mathbf{C}}_{jl}(\mathbf{g}) = \langle\mathbf{C}_{jl}(\mathbf{x})e^{-2\pi i\mathbf{g}\cdot\mathbf{x}}\rangle \tag{14}$$

and plugging it into $(11)_2$ yields the PWE formula for $\mathbf{C}_{jl}^{\mathrm{e}}$ as follows

$$\mathbf{C}_{jl}^{\mathrm{e}} = \widehat{\mathbf{C}}_{jl}(\mathbf{0}) - \mathbf{q}_j^+\mathbf{C}_0^{-1}\mathbf{q}_l, \ \ \text{where} \ \ \mathbf{q}_j = (g_i\widehat{\mathbf{C}}_{ij}(\mathbf{g}))_{\mathbf{g}\in\mathbb{Z}^3\setminus\mathbf{0}}, \ \ \mathbf{C}_0 = (g_k g_p'\widehat{\mathbf{C}}_{kp}(\mathbf{g}-\mathbf{g}'))_{\mathbf{g},\mathbf{g}'\in\mathbb{Z}^3\setminus\mathbf{0}}. \tag{15}$$

This result corresponds to the quasistatic limit of the effective elastic coefficients for a dynamically homogenized periodic medium, see [18, eq. (2.11)].

Unfortunately, although the PWE formula (15) is straightforward, its numerical use in 3D is complicated by the large algebraic dimensions of vectors and matrices of Fourier coefficients. This motivates using the monodromy matrix (MM) method which confines the PWE computation to 2D, see next Section. The MM method will also be shown to have significantly faster convergence than PWE.

3. MM formula

3.1. Derivation

The idea underlying the MM method is to reduce the 3-dimensional problem of Eq. $(11)_2$ to an equivalent 1-dimensional equation that can be integrated. This is achieved by focusing on a single coordinate and using Fourier transforms in the orthogonal coordinates. The MM formula may be deduced proceeding from Eq. $(11)_2$; using integration by parts, let us recast it into the form

$$\mathbf{C}^{\mathrm{e}}_{jl} = \langle \mathbf{C}_{jl} \rangle - \langle (\partial_p \mathbf{C}^{+}_{pj}) \mathbf{U} \rangle = \langle \mathbf{C}_{jp} \partial_p \mathbf{V} \rangle, \tag{16}$$

where we have denoted $\mathcal{C}_0^{-1}(\partial_q \mathbf{C}_{ql}) = \mathbf{U}$ and $\mathbf{V} = \mathbf{U} + x_l \mathbf{I}_3$ with $\mathbf{I}_3$ standing for the 3×3 identity matrix. Thus we need to solve the equation

$$\mathcal{C}_0 \mathbf{U} = \partial_q \mathbf{C}_{ql} \quad \Leftrightarrow \quad \mathcal{C}_0 \mathbf{U} = -\mathcal{C}_0 x_l \mathbf{I}_3 \quad \Leftrightarrow \quad \mathcal{C}_0 \mathbf{V} = 0 \quad \Leftrightarrow \quad \partial_q (\mathbf{C}_{qp} \partial_p \mathbf{V}) = 0 \text{ with } \mathbf{V} = \mathbf{U} + x_l \mathbf{I}_3. \tag{17}$$

In the following derivation the indices j, l are regarded as fixed, all repeated indices are summed and among them the indices a, b are specialized by the condition $a, b \neq l$. The suffix 0 of the differential operators $\boldsymbol{\mathcal{Q}}_0,\ \boldsymbol{\mathcal{M}}_0$ below indicates their reference to $\omega, k = 0$ (similarly to $\mathcal{C}_0$).

Equation (17) can be rewritten as an ordinary differential equation in the designated coordinate x_l

$$\boldsymbol{\Xi}' = \boldsymbol{\mathcal{Q}}_0\ \boldsymbol{\Xi} \quad \text{with} \quad ' \equiv \partial_l, \quad \boldsymbol{\Xi} = \begin{pmatrix} \mathbf{V} \\ \mathbf{C}_{lp} \partial_p \mathbf{V} \end{pmatrix}, \quad \boldsymbol{\mathcal{Q}}_0 = \begin{pmatrix} -\mathcal{B}^{-1} \mathcal{A}_1 & \mathcal{B}^{-1} \\ \mathcal{A}_2 - \mathcal{A}_1^{+} \mathcal{B}^{-1} \mathcal{A}_1 & \mathcal{A}_1^{+} \mathcal{B}^{-1} \end{pmatrix}, \tag{18}$$

where $\boldsymbol{\Xi}$ is a 6×3 matrix and the matrix operators $\mathcal{B}$, $\mathcal{A}_1$ and $\mathcal{A}_2$ are defined by

$$\mathcal{B} \mathbf{V} = \mathbf{C}_{ll} \mathbf{V}, \quad \mathcal{A}_1 \mathbf{V} = \mathbf{C}_{lb} \partial_b \mathbf{V}, \quad \mathcal{A}_2 \mathbf{V} = -\partial_a (\mathbf{C}_{ab} \partial_b \mathbf{V}). \tag{19}$$

Note that $\mathcal{B}$ and $\mathcal{A}_2$ are self-adjoint at any fixed x_l with respect to the inner product $(\cdot, \cdot)_{\bar{l}}$ (see (5)). Denote $\boldsymbol{\Xi}(s) \equiv \boldsymbol{\Xi}(\mathbf{x}) \mid_{x_l = s}$. The solution to (18) with some initial matrix function $\boldsymbol{\Xi}\,(0)$ has the form

$$\boldsymbol{\Xi}(x_l) = \boldsymbol{\mathcal{M}}_0(x_l)\, \boldsymbol{\Xi}\,(0) \quad \text{with } \boldsymbol{\mathcal{M}}_0(x_l) = \widehat{\int_0^{x_l}} (\boldsymbol{\mathcal{I}} + \boldsymbol{\mathcal{Q}}_0 dx_l), \tag{20}$$

where $\boldsymbol{\mathcal{M}}_0$ is a propagator matrix defined through the multiplicative integral $\widehat{\int}$ and $\boldsymbol{\mathcal{I}}$ is the identity operator. Note the identities

$$\text{for } \mathbf{W}_0 = \begin{pmatrix} \mathbf{I}_3 \\ \mathbf{0} \end{pmatrix}, \ \widetilde{\mathbf{W}}_0 = \begin{pmatrix} \mathbf{0} \\ \mathbf{I}_3 \end{pmatrix}: \quad \boldsymbol{\mathcal{Q}}_0 \mathbf{W}_0 = \mathbf{0}, \ \boldsymbol{\mathcal{Q}}_0^{+} \widetilde{\mathbf{W}}_0 = \mathbf{0} \quad \Rightarrow \quad \boldsymbol{\mathcal{M}}_0 \mathbf{W}_0 = \mathbf{W}_0, \ \boldsymbol{\mathcal{M}}_0^{+} \widetilde{\mathbf{W}}_0 = \widetilde{\mathbf{W}}_0. \tag{21}$$

It is seen that for any value of x_l the operator $\boldsymbol{\mathcal{M}}_0 - \boldsymbol{\mathcal{I}}$ has no inverse but at the same time it is a one-to-one mapping from the subspace orthogonal to $\mathbf{W}_0$ onto the subspace orthogonal to $\widetilde{\mathbf{W}}_0$. By the definitions of $\mathbf{V}$ and $\boldsymbol{\Xi}$ in (17), (18) and due to periodicity of $\mathbf{U}$, it follows that

$$\boldsymbol{\Xi}(1) = \boldsymbol{\Xi}(0) + \mathbf{W}_0 \ \Rightarrow \ \boldsymbol{\Xi}(0) = (\boldsymbol{\mathcal{M}}_0(1) - \boldsymbol{\mathcal{I}})^{-1} \mathbf{W}_0 \equiv \mathbf{S}. \tag{22}$$

Thus from (20), (22) and (18), (21),

$$\boldsymbol{\Xi}(x_l) = \boldsymbol{\mathcal{M}}_0(x_l) \mathbf{S} \quad \Rightarrow \quad \mathbf{V} = \mathbf{W}_0^{+} \boldsymbol{\mathcal{M}}_0(x_l) \mathbf{S}, \quad \mathbf{C}_{lp} \partial_p \mathbf{V} = \widetilde{\mathbf{W}}_0^{+} \boldsymbol{\mathcal{M}}_0(x_l) \mathbf{S}. \tag{23}$$

Substituting $\mathbf{V}$ obtained from (23) into (16) yields the desired formula for $\mathbf{C}^{\mathrm{e}}_{jl}$, which is discussed further in §3.2.3. Note, since $\boldsymbol{\mathcal{M}}$ is self-adjoint with respect to $(\cdot, \cdot)_{\bar{l}}$,

$$\langle \mathbf{C}_{lp} \partial_p \mathbf{V} \rangle_{\bar{l}} = (\boldsymbol{\mathcal{M}}_0(x_l) \mathbf{S}, \widetilde{\mathbf{W}}_0)_{\bar{l}} = (\mathbf{S}, \boldsymbol{\mathcal{M}}_0^{+}(x_l) \widetilde{\mathbf{W}}_0)_{\bar{l}} = (\mathbf{S}, \widetilde{\mathbf{W}}_0)_{\bar{l}} = \langle \widetilde{\mathbf{W}}_0^{+} \mathbf{S} \rangle_{\bar{l}}. \tag{24}$$

The latter identity implies that the laterally averaged 'traction' component of $\boldsymbol{\Xi}(x_l)$ is independent of x_l, and may be identified as a net 'force' acting on the faces x_l= constant.

Further simplification can be achieved for the matrices $\mathbf{C}_{ll}^{\text{eff}}$ $(= \mathbf{C}_{ll}^{\text{e}})$. By (16) and (58)

$$\mathbf{C}_{ll}^{\text{eff}} = \langle \mathbf{C}_{lp}\partial_p \mathbf{V}\rangle = \langle \widetilde{\mathbf{W}}_0^+ \mathbf{S}\rangle \equiv \langle \widetilde{\mathbf{W}}_0^+ (\boldsymbol{\mathcal{M}}_0(1) - \boldsymbol{\mathcal{I}})^{-1}\mathbf{W}_0\rangle_{\bar{l}}. \tag{25}$$

Equation (25) suffices to define the effective Christoffel tensor for $\mathbf{k} = k\kappa$ parallel to the translation vector $\mathbf{e}_l$ in which case $\mathbf{\Gamma}(\kappa) = \mathbf{C}_{ll}^{\text{eff}}$. Note that an alternative derivation of (25) is given in Appendix 1.

Finally it is noted that $\boldsymbol{\mathcal{M}}_0(1)$ which appears in the above expressions is formally a monodromy matrix (MM) relatively to the coordinate x_l, for which reason this approach and its outcome formulas are referred to as the MM ones. The MM approach to finding effective speed of shear (scalar) waves in 2D structures was first presented in [9], where Eq. (25) for vector waves was also mentioned but with neither derivation nor discussion.

3.2. Implementation

3.2.1. Propagator matrix in direction $\mathbf{e}_l$

As above, we fix l and keep $a, b \neq l$. Introduce the 2D Fourier expansion

$$\mathbf{C}_{pq}(\mathbf{x}) = \sum\nolimits_{\mathbf{g}\in\mathbb{Z}^2} e^{2\pi i g_a x_a}\widehat{\mathbf{C}}_{pq}(\mathbf{g}, x_l), \quad \widehat{\mathbf{C}}_{pq}(\mathbf{g}, x_l) = \langle \mathbf{C}_{pq}(\mathbf{x})e^{-2\pi i g_a x_a}\rangle_{\bar{l}}. \tag{26}$$

Operators $\mathcal{B}, \mathcal{A}_1, \mathcal{A}_2$ and matrix operators $\boldsymbol{\mathcal{Q}}, \boldsymbol{\mathcal{M}}_0(x_l)$ defined in (18)-(20) are represented in the 2D Fourier space by the following infinite matrices truncated to a finite size in calculations:

$$\mathcal{B} \mapsto \quad \mathbf{B} = (\widehat{\mathbf{C}}_{ll}(\mathbf{g}-\mathbf{g}', x_l))_{\mathbf{g},\mathbf{g}'\in\mathbb{Z}^2}, \tag{27a}$$

$$\mathcal{A}_1 \mapsto \quad \mathbf{A}_1 = 2\pi i(\widehat{\mathbf{C}}_{lb}(\mathbf{g}-\mathbf{g}', x_l)g_b')_{\mathbf{g},\mathbf{g}'\in\mathbb{Z}^2}, \tag{27b}$$

$$\mathcal{A}_2 \mapsto \quad \mathbf{A}_2 = 4\pi^2(g_a\widehat{\mathbf{C}}_{ab}(\mathbf{g}-\mathbf{g}', x_l)g_b')_{\mathbf{g},\mathbf{g}'\in\mathbb{Z}^2}, \tag{27c}$$

$$\boldsymbol{\mathcal{Q}}_0 \mapsto \quad \mathbf{Q}_0 = \begin{pmatrix} -\mathbf{B}^{-1}\mathbf{A}_1 & \mathbf{B}^{-1} \\ \mathbf{A}_2 - \mathbf{A}_1^+\mathbf{B}^{-1}\mathbf{A}_1 & \mathbf{A}_1^+\mathbf{B}^{-1} \end{pmatrix}, \tag{27d}$$

$$\boldsymbol{\mathcal{M}}_0(x_l) \mapsto \quad \mathbf{M}_0(x_l) = \widehat{\int_0^{x_l}}(\mathbf{I} + \mathbf{Q}_0 dx_l). \tag{27e}$$

3.2.2. Principal directions $\kappa \parallel \mathbf{e}_l$

Consider the effective matrices $\mathbf{C}_{ll}^{\text{eff}}$ $(= \mathbf{\Gamma}$ if $\kappa \parallel \mathbf{e}_l)$. In view of the above notations, formula (25) for $\mathbf{C}_{ll}^{\text{eff}}$ is expressed as

$$\mathbf{C}_{ll}^{\text{eff}} = \widetilde{\mathbf{W}}_{\widehat{0}}^+\widehat{\mathbf{S}} \ \text{ with } \ \widehat{\mathbf{S}} = (\mathbf{M}_0(1) - \mathbf{I})^{-1}\mathbf{W}_{\widehat{0}}, \tag{28}$$

where

$$\mathbf{W}_{\widehat{0}} = \begin{pmatrix} \mathbf{E}_{\widehat{0}} \\ \mathbf{0} \end{pmatrix}, \ \widetilde{\mathbf{W}}_{\widehat{0}} = \begin{pmatrix} \mathbf{0} \\ \mathbf{E}_{\widehat{0}} \end{pmatrix} \ \text{ with } \ \mathbf{E}_{\widehat{0}} = (\delta_{\mathbf{g0}}\mathbf{I}_3)_{\mathbf{g}\in\mathbb{Z}^2}. \tag{29}$$

Calculation of $\widehat{\mathbf{S}}$ in (28) can be performed by means of calculating $\mathbf{M}_0$ from its definition (27e), using any of the known methods for evaluating multiplicative integrals. However, this approach may suffer from numerical instabilities for $\mathbf{M}_0$ of large size due to exponential growth of some components of $\mathbf{M}_0$. Another method rests on calculating the resolvent $(\mathbf{M}_0 - \alpha\mathbf{I})^{-1}$ without calculating $\mathbf{M}_0$. The advantage of doing so is due to the fact that growing dimension of $\mathbf{M}_0$ leads to a relatively moderate growth of the resolvent components. Let us consider this latter method in some detail.

Denote the resolvent $\mathbf{R}_\alpha(x_l) = (\mathbf{M}_0(x_l) - \alpha\mathbf{I})^{-1}$ where α is not an eigenvalue of $\mathbf{M}_0(x_l)$. Since the matrix $\mathbf{M}_0(x_l)$ satisfies the differential equation $\mathbf{M}_0'(x_l) = \mathbf{Q}_0(x_l)\mathbf{M}_0(x_l)$ with the initial condition $\mathbf{M}_0(0) = \mathbf{I}$, it follows that $\mathbf{R}_\alpha(x_l)$ with a randomly chosen $\alpha \neq 1$ satisfies a Riccati equation with initial condition as follows

$$\begin{cases} \mathbf{R}_\alpha' = -\mathbf{R}_\alpha\mathbf{Q}_0(\mathbf{I} + \alpha\mathbf{R}_\alpha), \\ \mathbf{R}_\alpha(0) = (1-\alpha)^{-1}\mathbf{I}, \end{cases} \tag{30}$$

where $' = \partial_l$. Since eigenvalues of $\mathbf{M}_0$ usually tend to lie close to the real axis and unit circle, it is recommended to take $\alpha \in \mathbb{C}$ far from these sets. Integrating Eq. (30) numerically (we used the Runge-Kutta method of fourth order) provides $\mathbf{R}_\alpha(1) = (\mathbf{M}_0(1) - \alpha\mathbf{I})^{-1}$ where $\alpha \neq 1$. To exploit it for finding $\mathbf{C}^{\mathrm{eff}}_{ll}$ given by (28) we use the identity

$$\widehat{\mathbf{S}} \equiv (\mathbf{M}_0(1) - \mathbf{I})^{-1}\mathbf{W}_{\widehat{0}} = (\mathbf{I} + (\alpha-1)\mathbf{R}_\alpha(1))^{-1}\mathbf{R}_\alpha(1)\mathbf{W}_{\widehat{0}} = (\mathbf{I} + (\alpha-1)\mathbf{R}_\alpha(1))^{-1}\frac{\mathbf{W}_{\widehat{0}}}{1-\alpha}. \tag{31}$$

Thus $\widehat{\mathbf{S}}$ is found from the linear system

$$(1-\alpha)\big(\mathbf{I} + (\alpha-1)\mathbf{R}_\alpha(1)\big)\widehat{\mathbf{S}} = \mathbf{W}_{\widehat{0}}. \tag{32}$$

To solve (32), we first note that the matrix $\mathbf{T} \equiv (1-\alpha)\big(\mathbf{I} + (\alpha-1)\mathbf{R}_\alpha(1)\big)$ satisfies $\mathbf{T}\mathbf{W}_{\widehat{0}} = \mathbf{0}$, $\widetilde{\mathbf{W}}^+_{\widehat{0}}\mathbf{T} = \mathbf{0}$ with $\mathbf{W}_{\widehat{0}}$, $\widetilde{\mathbf{W}}_{\widehat{0}}$ from (29) and thus has 3 zero columns on the left of its vertical midline and 3 zero rows below the horizontal midline. Removing these columns and rows yields the reduced matrix $\widetilde{\mathbf{T}} = \begin{pmatrix} \mathbf{T}_1 & \mathbf{T}_2 \\ \mathbf{T}_3 & \mathbf{T}_4 \end{pmatrix}$ where the square block $\mathbf{T}_3$ has 3 rows and 3 columns less than the block $\mathbf{T}_2$. Since $\mathbf{T}_3$ is numerically large, while $\mathbf{T}_1, \mathbf{T}_4$ are medium and $\mathbf{T}_2$ small, it is convenient to apply Schur's formula to arrive at the final relation in the form

$$\mathbf{C}^{\mathrm{eff}}_{ll} = \mathbf{E}^+_{\widehat{0}}\big(\mathbf{T}_2 - \mathbf{T}_1\mathbf{T}_3^{-1}\mathbf{T}_4\big)^{-1}\mathbf{E}_{\widehat{0}}. \tag{33}$$

3.2.3. Off-principal directions

Consider $\mathbf{k} = k\kappa$ of arbitrary orientation relatively to the translations $\mathbf{e}_l$. In order to find the effective Christoffel tensor $\mathbf{\Gamma}(\kappa)$ of Eq. (12) for arbitrary κ ($\nparallel \mathbf{e}_l$), we need to calculate $\mathbf{C}^{\mathrm{e}}_{jl}$ with $j \neq l$. Applying the 2D Fourier expansion to Eqs. (16) and (23) yields

$$\mathbf{C}^{\mathrm{e}}_{jl} = \langle \mathbf{E}^+_{\widehat{0}}\,(\mathbf{A}_1 + \overline{\mathbf{C}}_{jl}\partial_l)\widehat{\mathbf{V}}\rangle_l = \mathbf{C}^{\mathrm{eff}}_{ll} + \langle \mathbf{E}^+_{\widehat{0}}\,(\overline{\mathbf{C}}_{ll} - \overline{\mathbf{C}}_{jl})\mathbf{B}^{-1}(\mathbf{A}_1\widehat{\mathbf{V}} - \widehat{\mathbf{N}})\rangle_l, \text{ where } \begin{pmatrix}\widehat{\mathbf{V}} \\ \widehat{\mathbf{N}}\end{pmatrix} = \mathbf{M}_0(x_l)\widehat{\mathbf{S}} \tag{34}$$

and $\overline{\mathbf{C}}_{jp} = (\widehat{\mathbf{C}}_{jp}(\mathbf{g} - \mathbf{g}', x_l))_{\mathbf{g},\mathbf{g}' \in \mathbb{Z}^2}$ with $\mathbf{g} = (g_a\, g_b)$ and $a, b \neq l$. As detailed above, the matrix $\widehat{\mathbf{S}}$ can be calculated with a very good precision. Evaluation of $\widehat{\mathbf{V}}(x_l)$ and $\widehat{\mathbf{N}}(x_l)$ is no longer that accurate, particularly for high-contrast structures which require many terms in the Fourier series and hence need $\mathbf{M}_0$ of large algebraic dimension and therefore with large values of some components. Thus a negligible error in $\mathbf{S}$ may become noticeable after multiplying by $\mathbf{M}_0$. In this regard, we present an alternative method of calculating $\mathbf{C}^{\mathrm{e}}_{jl}$ with $j \neq l$ which circumvents (34).

For the fixed functions $\rho(\mathbf{x})$ and $c_{ijkl}(\mathbf{x})$ with a given cubic lattice of periods $\mathbf{e}_p = (\delta_{pq})$, introduce the new periods $\mathbf{a}_p = \mathbf{A}\mathbf{e}_p$ where $\mathbf{A}$ has integer components a_{ij}. The solutions $\mathbf{v}(\mathbf{x}) = \mathbf{u}(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}}$ and $\omega(\mathbf{k})$ of the wave equation (3) remain unaltered, as they do not depend on the choice of periods. But now in order to define $\mathbf{C}^{\mathrm{eff}}_{jl}$ by the MM formula (which requires periods to coincide with base vectors) we should apply the change of variables $\mathbf{x} \to \mathbf{A}\mathbf{x}$ that leads, as explained in §3.3, to new functions for the density and elasticity with the periods $\mathbf{e}_p = (\delta_{pq})$. According to Eqs. (49) and (56) of §3.3,

$$\mathbf{C}^{\mathrm{eff}}_{pq} = a_{pj}\widetilde{\mathbf{C}}^{\mathrm{eff}}_{jl}a_{ql} = a_{pj}\mathbf{A}\overline{\mathbf{C}}^{\mathrm{eff}}_{jl}\mathbf{A}^+a_{ql} \quad \Big(\Leftrightarrow\ \widetilde{\mathbf{C}}^{\mathrm{eff}}_{jl} = b_{jp}\mathbf{C}^{\mathrm{eff}}_{pq}b_{lq},\ \overline{\mathbf{C}}^{\mathrm{eff}}_{jl} = b_{jp}\mathbf{B}\mathbf{C}^{\mathrm{eff}}_{pq}\mathbf{B}^+b_{lq}\Big) \tag{35}$$

where $\widetilde{\mathbf{C}}^{\mathrm{eff}}_{jl}$ and $\overline{\mathbf{C}}^{\mathrm{eff}}_{jl}$ are the effective matrices associated with the new profiles $\widetilde{c}_{ijkl}(\mathbf{x}) = b_{jp}b_{lq}c_{ipkq}(\mathbf{A}\mathbf{x})$ and $\overline{c}_{ijkl}(\mathbf{x}) = b_{im}b_{jp}b_{kn}b_{lq}c_{mpnq}(\mathbf{A}\mathbf{x})$, respectively, and b_{ij} stand for components of $\mathbf{A}^{-1}$. We may apply (35) successively for each of the transformations $\mathbf{a}_p = \mathbf{A}_j\mathbf{e}_p$, $j = 1, 2, 3$,

$$\mathbf{A}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 1 & 1 \end{pmatrix} \Leftrightarrow \begin{matrix} \mathbf{a}_1 = \mathbf{e}_1, \\ \mathbf{a}_2 = \mathbf{e}_2 + \mathbf{e}_3, \\ \mathbf{a}_3 = -\mathbf{e}_2 + \mathbf{e}_3, \end{matrix} \quad \mathbf{A}_2 = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix} \Leftrightarrow ..., \ \mathbf{A}_3 = \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \Leftrightarrow ... . \tag{36}$$

Using the inverse forms in (35) leads to a variety of identities, for instance,

$$\begin{aligned}
\mathbf{C}_{23}^{\text{eff}} + \mathbf{C}_{32}^{\text{eff}} &= 4(\widetilde{\mathbf{C}}_{22}^{\text{eff}})_{\mathbf{A}_1} - \mathbf{C}_{22}^{\text{eff}} - \mathbf{C}_{33}^{\text{eff}} = 4(\mathbf{A}\overline{\mathbf{C}}_{22}^{\text{eff}}\mathbf{A}^+)_{\mathbf{A}_1} - \mathbf{C}_{22}^{\text{eff}} - \mathbf{C}_{33}^{\text{eff}}, \\
\mathbf{C}_{31}^{\text{eff}} + \mathbf{C}_{13}^{\text{eff}} &= 4(\widetilde{\mathbf{C}}_{33}^{\text{eff}})_{\mathbf{A}_2} - \mathbf{C}_{33}^{\text{eff}} - \mathbf{C}_{11}^{\text{eff}} = 4(\mathbf{A}\overline{\mathbf{C}}_{33}^{\text{eff}}\mathbf{A}^+)_{\mathbf{A}_2} - \mathbf{C}_{33}^{\text{eff}} - \mathbf{C}_{11}^{\text{eff}}, \\
\mathbf{C}_{12}^{\text{eff}} + \mathbf{C}_{21}^{\text{eff}} &= 4(\widetilde{\mathbf{C}}_{11}^{\text{eff}})_{\mathbf{A}_3} - \mathbf{C}_{11}^{\text{eff}} - \mathbf{C}_{22}^{\text{eff}} = 4(\mathbf{A}\overline{\mathbf{C}}_{11}^{\text{eff}}\mathbf{A}^+)_{\mathbf{A}_3} - \mathbf{C}_{11}^{\text{eff}} + \mathbf{C}_{22}^{\text{eff}}.
\end{aligned} \tag{37}$$

Inserting (37) in (12) eliminates $\mathbf{C}_{jl}^{\text{eff}} + \mathbf{C}_{lj}^{\text{eff}}$ with $j \neq l$ and expresses the effective Christoffel tensor $\mathbf{\Gamma}$ fully in terms of the matrices $\mathbf{C}_{ll}^{\text{eff}}$ and either of $(\widetilde{\mathbf{C}}_{ll}^{\text{eff}})_{\mathbf{A}_n}$ or $(\overline{\mathbf{C}}_{ll}^{\text{eff}})_{\mathbf{A}_n}$ $(n = 1, 2, 3)$, which are defined by Eqs. (25), (28) with $c_{ijkl}(\mathbf{x})$ replaced by $\widetilde{c}_{ijkl}(\mathbf{x})$ or $\overline{c}_{ijkl}(\mathbf{x})$, respectively. Thus all calculations have been reduced to the form (28) which ensures a numerically stable evaluation of $\mathbf{\Gamma}$.

Note that the transformed elasticity $\overline{c}_{ijkl}(\mathbf{x})$ retains the usual symmetries under the interchange of indices, while $\widetilde{c}_{ijkl}(\mathbf{x})$ does not (see §3.3). Also, the transformations defined by (36) for the cubic unit cell can be identified as rotations by virtue of the fact that $\frac{1}{\sqrt{2}}\mathbf{A}_j$, $j = 1, 2, 3$, are orthogonal matrices of unit determinant. Hence, apart from a factor of $\frac{1}{4}$, $\left(\overline{c}_{ijkl}(\mathbf{x})\right)_{\mathbf{A}_j}$ is precisely the elasticity tensor represented in a coordinate system rotated about the axis $\mathbf{e}_j$ by $\frac{\pi}{4}$ from the original.

3.3. The case of an oblique lattice

3.3.1. Equivalent problem on a cubic lattice

Consider the problem of quasistatic asymptotics of the wave equation (3) for the general case of a 3D periodic elastic medium with

$$\rho(\mathbf{x}) = \rho\left(\mathbf{x} + \mathbf{a}_p\right), \; c_{ijkl}(\mathbf{x}) = c_{ijkl}\left(\mathbf{x} + \mathbf{a}_p\right), \tag{38}$$

where the translation vectors $\mathbf{a}_p$ form an oblique lattice. We will define the solution of this problem via the solution for a simpler case of a cubic lattice.

The oblique lattice vectors are defined by a matrix $\mathbf{A}$ $(\neq \mathbf{I})$ as

$$\mathbf{a}_p = \mathbf{A}\mathbf{e}_p \text{ with } \mathbf{A} = (a_{pq})_{p,q=1}^3 = (\mathbf{a}_p \cdot \mathbf{e}_q)_{p,q=1}^3 \,; \; \mathbf{B} \equiv \mathbf{A}^{-1} = (b_{pq})_{p,q=1}^3 \tag{39}$$

where $\mathbf{e}_p$ are the orthonormal vectors used previously. Define the new or transformed position variable $\mathbf{x}' = \mathbf{B}\mathbf{x}$ $(\Leftrightarrow \mathbf{x} = \mathbf{A}\mathbf{x}')$, the associated displacement $\widetilde{\mathbf{v}}(\mathbf{x}') = \mathbf{v}(\mathbf{x})$ and material parameters $\widetilde{\rho}(\mathbf{x}') = \rho(\mathbf{x})$, $c_{ijkl}^{(1)}(\mathbf{x}') = c_{ijkl}(\mathbf{x})$, which are seen to be periodic in $\mathbf{x}'$ with respect to the vectors $\mathbf{e}_p$. Setting $\mathbf{C}_{jl}^{(1)} = \left(c_{ijkl}^{(1)}\right)_{i,k=1}^3$, the equation of motion (3) becomes

$$b_{jp}b_{lq}\,\partial_{j'}\left(\mathbf{C}_{pq}^{(1)}\partial_{l'}\widetilde{\mathbf{v}}\right) = -\widetilde{\rho}\omega^2\widetilde{\mathbf{v}}, \tag{40}$$

where $\partial_{j'} \equiv \partial/\partial x_j'$. Using the fact that $\mathbf{B}$ is constant allows it to be removed explicitly from (40) by incorporation into a newly defined stiffness tensor. Thus, replacing $\mathbf{x}' \to \mathbf{x}$ we have

$$\partial_j(\widetilde{\mathbf{C}}_{jl}\partial_l\widetilde{\mathbf{v}}) = -\widetilde{\rho}\omega^2\widetilde{\mathbf{v}}, \tag{41}$$

where $\widetilde{\mathbf{v}}(\mathbf{x}) = \mathbf{v}(\mathbf{A}\mathbf{x})$ and the material parameters are

$$\begin{aligned}
\widetilde{\rho}(\mathbf{x}) &= \rho(\mathbf{A}\mathbf{x}) \quad (= \widetilde{\rho}(\mathbf{x} + \mathbf{e}_p)), \\
\widetilde{c}_{ijkl}(\mathbf{x}) &= b_{jp}b_{lq}c_{ipkq}(\mathbf{A}\mathbf{x}) \quad (= \widetilde{c}_{ijkl}(\mathbf{x} + \mathbf{e}_p)), \\
\widetilde{\mathbf{C}}_{jl}(\mathbf{x}) &= (\widetilde{c}_{ijkl})_{i,k=1}^3 = b_{jp}b_{lq}\mathbf{C}_{pq}(\mathbf{A}\mathbf{x}) = \widetilde{\mathbf{C}}_{lj}^+(\mathbf{x}),
\end{aligned} \tag{42}$$

which are periodic in $\mathbf{x}$ with respect to the cubic lattice formed by vectors $\mathbf{e}_p$. Note that the tensor $\widetilde{c}_{ijkl}$ for $\mathbf{A} \neq \mathbf{I}$ is of Cosserat type in that it is not invariant to permutations of indices $i \rightleftarrows j$ and $k \rightleftarrows l$ but retains the major symmetry $\widetilde{c}_{ijkl} = \widetilde{c}_{klij}^*$ $(= \widetilde{c}_{klij}$ for real case).

The Floquet condition $\mathbf{v}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}\mathbf{u}(\mathbf{x})$ with periodic $\mathbf{u}(\mathbf{x}) = \mathbf{u}(\mathbf{x}+\mathbf{a}_j)$ satisfying

$$-(\partial_l + ik_l)\mathbf{C}_{lq}(\partial_q + ik_q)\mathbf{u} = \rho\omega^2\mathbf{u} \tag{43}$$

is equivalent to the condition $\widetilde{\mathbf{v}}(\mathbf{x}) = e^{i\widetilde{\mathbf{k}}\cdot\mathbf{x}}\widetilde{\mathbf{u}}(\mathbf{x})$with periodic $\widetilde{\mathbf{u}}(\mathbf{x})$ satisfying the equation that follows from (40),

$$-(\partial_l + i\widetilde{k}_l)\widetilde{\mathbf{C}}_{lq}(\partial_q + i\widetilde{k}_q)\widetilde{\mathbf{u}} = \widetilde{\rho}\widetilde{\omega}^2\widetilde{\mathbf{u}}, \tag{44}$$

where

$$\widetilde{\mathbf{k}} = \mathbf{A}^+\mathbf{k}\ (=\widetilde{k}\widetilde{\kappa},\ |\widetilde{\kappa}|=1),\quad \widetilde{\omega}(\widetilde{\mathbf{k}}) = \omega(\mathbf{k}),\quad \widetilde{\mathbf{u}}(\mathbf{x}) = \mathbf{u}(\mathbf{A}\mathbf{x})\ \ (=\widetilde{\mathbf{u}}(\mathbf{x}+\mathbf{e}_p))\,. \tag{45}$$

Equation (44), which is defined on a cubic lattice, has quasistatic asymptotics as described above. According to (10),

$$\widetilde{\mathbf{\Gamma}}\widetilde{\mathbf{u}}_{0\alpha} = \langle\widetilde{\rho}\rangle\widetilde{c}_\alpha^2\widetilde{\mathbf{u}}_{0\alpha} \text{ with } \widetilde{c}_\alpha(\widetilde{\boldsymbol{\kappa}}) \equiv \lim_{\widetilde{k}\to 0}\widetilde{\omega}_\alpha(\widetilde{\mathbf{k}})/\widetilde{k},\ \alpha = 1,2,3, \tag{46}$$

where $\widetilde{\mathbf{\Gamma}}(\widetilde{\boldsymbol{\kappa}}) = \widetilde{\kappa}_j\widetilde{\kappa}_l\widetilde{\mathbf{C}}_{jl}^{\text{eff}}$. Let us write a similar relation for the quasistatic asymptotics of (43),

$$\mathbf{\Gamma}\mathbf{u}_{0\alpha} = \langle\rho\rangle c_\alpha^2\mathbf{u}_{0\alpha} \text{ with } c_\alpha(\boldsymbol{\kappa}) \equiv \lim_{k\to 0}\omega_\alpha(\mathbf{k})/k, \tag{47}$$

where $\mathbf{k} = k\boldsymbol{\kappa}$ ($|\boldsymbol{\kappa}| = 1$) and $\mathbf{\Gamma}(\boldsymbol{\kappa})$ is to be determined. Comparing (46) and (47) with regard for (45) and making use of the equality $\langle\widetilde{\rho}\rangle \equiv \int_{[0,1]^3}\rho(\mathbf{A}\mathbf{x})d\mathbf{x} = \langle\rho\rangle$, we find that

$$\frac{1}{\langle\rho\rangle}k^2\mathbf{\Gamma} = \frac{1}{\langle\widetilde{\rho}\rangle}\widetilde{k}^2\widetilde{\mathbf{\Gamma}} \ \Rightarrow\ \mathbf{\Gamma} = \frac{\langle\rho\rangle}{\langle\widetilde{\rho}\rangle}\frac{\widetilde{k}_j\widetilde{k}_l}{k^2}\widetilde{\mathbf{C}}_{jl}^{\text{eff}} = \kappa_p a_{pj}\widetilde{\mathbf{C}}_{jl}^{\text{eff}}a_{ql}\kappa_q \tag{48}$$

and hence

$$\mathbf{\Gamma}(\boldsymbol{\kappa}) = \mathbf{C}_{pq}^{\text{eff}}\kappa_p\kappa_q:\quad \mathbf{C}_{pq}^{\text{eff}} = a_{pj}\widetilde{\mathbf{C}}_{jl}^{\text{eff}}a_{ql}\ \ \Big(\Leftrightarrow\ \widetilde{\mathbf{C}}_{jl}^{\text{eff}} = b_{jp}\mathbf{C}_{pq}^{\text{eff}}b_{lq}\Big). \tag{49}$$

3.3.2. Alternative formulation using anisotropic mass density

Premultiplication of Eq. (41) by $\mathbf{B}$ allows it to be reformulated as

$$\partial_j(\overline{\mathbf{C}}_{jl}\partial_l\overline{\mathbf{v}}) = -\overline{\boldsymbol{\rho}}\omega^2\overline{\mathbf{v}}, \tag{50}$$

where $\overline{\mathbf{v}}$ and the material parameters are

$$\begin{aligned}
\overline{\mathbf{v}}(\mathbf{x}) &= \mathbf{A}^+\mathbf{v}(\mathbf{A}\mathbf{x})\ \ \big(=\mathbf{A}^+\widetilde{\mathbf{v}}(\mathbf{x})\big),\\
\overline{\boldsymbol{\rho}}(\mathbf{x}) &= \mathbf{B}\mathbf{B}^+\rho(\mathbf{A}\mathbf{x}) = \mathbf{B}\mathbf{B}^+\widetilde{\rho}(\mathbf{x}) = \overline{\boldsymbol{\rho}}^+(\mathbf{x})\quad (=\overline{\rho}(\mathbf{x}+\mathbf{e}_p))\,,\\
\overline{c}_{ijkl}(\mathbf{x}) &= b_{im}b_{jp}b_{kn}b_{lq}c_{mpnq}(\mathbf{A}\mathbf{x})\quad (=\overline{c}_{ijkl}(\mathbf{x}+\mathbf{e}_p))\,,\\
\overline{\mathbf{C}}_{jl}(\mathbf{x}) &= (\overline{c}_{ijkl})_{i,k=1}^3 = b_{jp}b_{lq}\mathbf{B}\mathbf{C}_{pq}(\mathbf{A}\mathbf{x})\mathbf{B}^+ = \mathbf{B}\widetilde{\mathbf{C}}_{pq}(\mathbf{x})\mathbf{B}^+ = \overline{\mathbf{C}}_{lj}^+(\mathbf{x}),
\end{aligned} \tag{51}$$

which are periodic in $\mathbf{x}$ with respect to the cubic lattice of vectors $\mathbf{e}_p$. Note that the tensor $\overline{c}_{ijkl}$ retains the major and minor symmetries of normal elasticity, $\overline{c}_{ijkl} = \overline{c}_{klij}^*$ and $\overline{c}_{ijkl} = \overline{c}_{jikl}$, while the mass density is no longer a scalar but becomes a symmetric tensor.

The Floquet condition now becomes $\overline{\mathbf{v}}(\mathbf{x}) = e^{i\overline{\mathbf{k}}\cdot\mathbf{x}}\overline{\mathbf{u}}(\mathbf{x})$ with periodic $\overline{\mathbf{u}}(\mathbf{x})$ satisfying

$$-(\partial_l + i\overline{k}_l)\overline{\mathbf{C}}_{lq}(\partial_q + i\overline{k}_q)\overline{\mathbf{u}} = \overline{\boldsymbol{\rho}}\,\overline{\omega}^2\overline{\mathbf{u}}, \tag{52}$$

where

$$\overline{\mathbf{k}} = \mathbf{A}^+\mathbf{k}\ (=\overline{k}\overline{\kappa},\ |\overline{\kappa}|=1),\quad \overline{\omega}(\overline{\mathbf{k}}) = \omega(\mathbf{k}),\quad \overline{\mathbf{u}}(\mathbf{x}) = \mathbf{A}^+\mathbf{u}(\mathbf{A}\mathbf{x})\ \ (=\overline{\mathbf{u}}(\mathbf{x}+\mathbf{e}_p))\,. \tag{53}$$

Its quasistatic asymptotics are

$$\overline{\mathbf{\Gamma}}\overline{\mathbf{u}}_{0\alpha} = \langle\overline{\boldsymbol{\rho}}\rangle\overline{c}_\alpha^2\overline{\mathbf{u}}_{0\alpha} \text{ with } \overline{c}_\alpha(\overline{\boldsymbol{\kappa}}) \equiv \lim_{k\to 0}\overline{\omega}_\alpha(\overline{\mathbf{k}})/\overline{k},\ \alpha = 1,2,3, \tag{54}$$

where $\overline{\mathbf{\Gamma}}(\overline{\boldsymbol{\kappa}}) = \overline{\kappa}_j\overline{\kappa}_l\overline{\mathbf{C}}_{jl}^{\text{eff}}$. Comparing (47) and (54) with regard for (53) and making use of the equality $\langle\overline{\boldsymbol{\rho}}\rangle = \mathbf{B}\mathbf{B}^+\langle\widetilde{\rho}\rangle = \mathbf{B}\mathbf{B}^+\langle\rho\rangle$, we find that

$$\langle\rho\rangle^{-1}k^2\mathbf{\Gamma} = \langle\rho\rangle^{-1}\overline{k}^2\mathbf{A}\overline{\mathbf{\Gamma}}\mathbf{A}^+ \ \Rightarrow\ \mathbf{\Gamma} = \kappa_p a_{pj}\mathbf{A}\overline{\mathbf{C}}_{jl}^{\text{eff}}\mathbf{A}^+a_{ql}\kappa_q \tag{55}$$

and hence

$$\mathbf{C}_{pq}^{\text{eff}} = a_{pj}\mathbf{A}\overline{\mathbf{C}}_{jl}^{\text{eff}}\mathbf{A}^+a_{ql} \quad \Big(\Leftrightarrow\ \overline{\mathbf{C}}_{jl}^{\text{eff}} = b_{jp}\mathbf{B}\mathbf{C}_{pq}^{\text{eff}}\mathbf{B}^+b_{lq}\Big). \tag{56}$$

3.3.3. Summary of the oblique case

Given material constants $\rho(\mathbf{x})$ and $c_{ijkl}(\mathbf{x})$ on an oblique lattice we first identify the matrix $\mathbf{A}$ of (39). We may proceed in either of two ways based on Cosserat elasticity with isotropic density, or normal elasticity with anisotropic density. In each case we define material properties on a cubic lattice: $\widetilde{\rho}(\mathbf{x})$, $\widetilde{\mathbf{C}}_{jl}(\mathbf{x})$ from Eq. (42) or $\overline{\boldsymbol{\rho}}(\mathbf{x})$, $\overline{\mathbf{C}}_{jl}(\mathbf{x})$ from Eq. (51), respectively. Then use the formulas of §3 to obtain $\widetilde{\mathbf{C}}_{jl}(\mathbf{x}) \to \widetilde{\mathbf{C}}_{jl}^{\text{eff}}$ or $\overline{\mathbf{C}}_{jl}(\mathbf{x}) \to \overline{\mathbf{C}}_{jl}^{\text{eff}}$, and finally insert the result into (49) or (56) to arrive at the sought effective Christoffel matrix $\mathbf{\Gamma}$ as a function of unit direction vector $\boldsymbol{\kappa}$ in the oblique lattice. Knowing $\mathbf{\Gamma}(\boldsymbol{\kappa})$ yields the effective speeds $c_\alpha(\boldsymbol{\kappa})$ according to (47). Note that although the formulation in §2 was restricted to isotropic density, the quasi-static effective elasticity is the same if one replaces the isotropic density tensor $\rho(\mathbf{x})\mathbf{I}$ by the anisotropic density $\rho(\mathbf{x})\mathbf{J}$ with $\mathbf{J} = \mathbf{J}^+$ constant positive definite. In the case of the anisotropic density formulation for the oblique lattice $\mathbf{J} = \mathbf{B}\mathbf{B}^+$.

3.4. Calculating the effective elastic moduli.

We return to the question of the full determination of c_{ijkl}^{eff} from the Christoffel tensor, or more specifically, from $\mathbf{D}$ defined by

$$d_{ikjl} = \frac{1}{2}\big(c_{ijkl}^{\text{eff}} + c_{ilkj}^{\text{eff}}\big). \tag{57}$$

The elements of $\mathbf{D}$ satisfy the same symmetries as those of $\mathbf{C}$ ($d_{ikjl} = d_{jlik} = d_{iklj}$) and they follow from Eq. (13) as

$$(d_{ikjl})_{i,k=1}^3 = \frac{1}{2}\big(\mathbf{C}_{jl}^{\text{eff}} + \mathbf{C}_{lj}^{\text{eff}}\big) = \frac{1}{2}\big(\mathbf{C}_{jl}^{\text{e}} + \mathbf{C}_{lj}^{\text{e}}\big) \equiv \mathbf{D}_{jl} \ \ \big(= \mathbf{D}_{lj}\big). \tag{58}$$

Define the 'totally symmetric' part of $\mathbf{C}^{\text{eff}}$ as $c_{ijkl}^{\text{eff,s}} = \frac{1}{3}\big(c_{ijkl}^{\text{eff}} + c_{ikjl}^{\text{eff}} + c_{iljk}^{\text{eff}}\big)$. This is seen to be equal to the totally symmetric part of $\mathbf{D}$ defined in (57), i.e. $\mathbf{C}^{\text{eff,s}} = \mathbf{D}^{\text{s}}$ where $d_{ijkl}^{\text{s}} = \frac{1}{3}\big(d_{ijkl} + d_{ikjl} + d_{iljk}\big)$. Equation (57) can then be rewritten as [19]

$$\mathbf{D} = \frac{3}{2}\mathbf{C}^{\text{eff,s}} - \frac{1}{2}\mathbf{C}^{\text{eff}} \ \Rightarrow\ \mathbf{C}^{\text{eff}} = 3\mathbf{D}^{\text{s}} - 2\mathbf{D}. \tag{59}$$

The latter inverse relation may be simply represented in Voigt notation as

$$\begin{pmatrix} c_{11}^{\text{eff}} & c_{12}^{\text{eff}} & c_{13}^{\text{eff}} & c_{14}^{\text{eff}} & c_{15}^{\text{eff}} & c_{16}^{\text{eff}} \\ & c_{22}^{\text{eff}} & c_{23}^{\text{eff}} & c_{24}^{\text{eff}} & c_{25}^{\text{eff}} & c_{26}^{\text{eff}} \\ & & c_{33}^{\text{eff}} & c_{34}^{\text{eff}} & c_{35}^{\text{eff}} & c_{36}^{\text{eff}} \\ & & & c_{44}^{\text{eff}} & c_{45}^{\text{eff}} & c_{46}^{\text{eff}} \\ S & Y & M & & c_{55}^{\text{eff}} & c_{56}^{\text{eff}} \\ & & & & & c_{66}^{\text{eff}} \end{pmatrix} = \begin{pmatrix} d_{11} & 2d_{66}-d_{12} & 2d_{55}-d_{13} & 2d_{56}-d_{14} & d_{15} & d_{16} \\ & d_{22} & 2d_{44}-d_{23} & d_{24} & 2d_{46}-d_{25} & d_{26} \\ & & d_{33} & d_{34} & d_{35} & 2d_{45}-d_{36} \\ & & & d_{23} & d_{36} & d_{25} \\ & SYM & & & d_{13} & d_{14} \\ & & & & & d_{12} \end{pmatrix}. \tag{60}$$

This one-to-one correspondence between the elements $\mathbf{C}^{\text{eff}}$ and $\mathbf{D}$, combined with the identity (58), provides the means to find the effective moduli from $\mathbf{C}_{jl}^{\text{e}}$.

It remains to determine the full set of elements d_{ijkl} from Christoffel tensors for a given set of directions. It is known that data for at least six distinct directions are required [20, 21]. The necessary and sufficient condition that a given sextet $\{\mathbf{\Gamma}^{(\alpha)} \equiv \mathbf{\Gamma}(\boldsymbol{\kappa}^{\alpha}), \alpha = 1,..,6\}$ will yield the full elastic moduli tensor is that the six directions $\{\boldsymbol{\kappa}^{\alpha}\}$ do not lie on a cone through the origin and cannot be contained in less than three distinct planes through the origin [21]. The set $\{\boldsymbol{\kappa}^{\alpha}\} = \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \frac{1}{\sqrt{2}}\mathbf{A}_1\mathbf{e}_2, \frac{1}{\sqrt{2}}\mathbf{A}_2\mathbf{e}_3, \frac{1}{\sqrt{2}}\mathbf{A}_3\mathbf{e}_1\}$ (see (36)) meets this requirement (and is in fact the set first proposed in [20]). Thus the complete set of d_{ijkl} follows from [21, Eq. (3.17)] (see Eq. (58))

$$\mathbf{D}_{jl} = \sum_{\alpha=1}^{3} \mathbf{\Gamma}^{(\alpha)} \big(\kappa_j^{\alpha}\kappa_l^{\alpha} - \tfrac{1}{\sqrt{2}}(\kappa_j^{\alpha+3}\kappa_l^{\alpha} + \kappa_j^{\alpha}\kappa_l^{\alpha+3})\big) + \sum_{\substack{\alpha,\beta=1\\ \beta>\alpha}}^{3} \mathbf{\Gamma}^{(9-\alpha-\beta)}(\kappa_j^{\alpha}\kappa_l^{\beta} + \kappa_j^{\beta}\kappa_l^{\alpha}). \tag{61}$$

The equivalent form of (61) in Voigt notation is

$$\begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\ & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\ & & d_{33} & d_{34} & d_{35} & d_{36} \\ & & & d_{44} & d_{45} & d_{46} \\ S & Y & M & & d_{55} & d_{56} \\ & & & & & d_{66} \end{pmatrix} = \begin{pmatrix} \Gamma_{11}^{(1)} & \Gamma_{11}^{(2)} & \Gamma_{11}^{(3)} & \Gamma_{11}^{(4)} & \Gamma_{11}^{(5)} & \Gamma_{11}^{(6)} \\ \Gamma_{22}^{(1)} & \Gamma_{22}^{(2)} & \Gamma_{22}^{(3)} & \Gamma_{22}^{(4)} & \Gamma_{22}^{(5)} & \Gamma_{22}^{(6)} \\ \Gamma_{33}^{(1)} & \Gamma_{33}^{(2)} & \Gamma_{33}^{(3)} & \Gamma_{33}^{(4)} & \Gamma_{33}^{(5)} & \Gamma_{33}^{(6)} \\ \Gamma_{23}^{(1)} & \Gamma_{23}^{(2)} & \Gamma_{23}^{(3)} & \Gamma_{23}^{(4)} & \Gamma_{23}^{(5)} & \Gamma_{23}^{(6)} \\ \Gamma_{31}^{(1)} & \Gamma_{31}^{(2)} & \Gamma_{31}^{(3)} & \Gamma_{31}^{(4)} & \Gamma_{31}^{(5)} & \Gamma_{31}^{(6)} \\ \Gamma_{12}^{(1)} & \Gamma_{12}^{(2)} & \Gamma_{12}^{(3)} & \Gamma_{12}^{(4)} & \Gamma_{12}^{(5)} & \Gamma_{12}^{(6)} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 & -\frac{1}{2} & -\frac{1}{2} \\ 0 & 1 & 0 & -\frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & 0 & 1 & -\frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{62}$$

The full set of c_{ijkl}^{eff} can therefore be obtained from Eqs. (60) and (62) with (see Eq. (37))

$$\begin{aligned} &\mathbf{\Gamma}^{(1)} = \mathbf{C}_{11}^{\text{eff}}, && \mathbf{\Gamma}^{(2)} = \mathbf{C}_{22}^{\text{eff}}, && \mathbf{\Gamma}^{(3)} = \mathbf{C}_{33}^{\text{eff}}, \\ &\mathbf{\Gamma}^{(4)} = 2(\mathbf{A}\overline{\mathbf{C}}_{22}^{\text{eff}}\mathbf{A}^{+})_{\mathbf{A}_1}, && \mathbf{\Gamma}^{(5)} = 2(\mathbf{A}\overline{\mathbf{C}}_{33}^{\text{eff}}\mathbf{A}^{+})_{\mathbf{A}_2}, && \mathbf{\Gamma}^{(6)} = 2(\mathbf{A}\overline{\mathbf{C}}_{11}^{\text{eff}}\mathbf{A}^{+})_{\mathbf{A}_3}. \end{aligned} \tag{63}$$

Other procedures for inverting a set of compatible Christoffel tensors to give the moduli can be found in [21].

4. Closed-form upper bound of the effective Christoffel tensor

Let $N \geq 0$ be the truncation parameter of the 3D or 2D Fourier expansion of $\mathbf{C}_{jl}(\mathbf{x})$, meaning that the index $\mathbf{g}$ in (14) or (26) takes the values from the set $[-N, N]^3$ or $[-N, N]^2$, respectively. Denote truncated approximations of the effective Christoffel tensor $\mathbf{\Gamma}(\kappa) = \mathbf{C}_{jl}^{\text{eff}}\kappa_j\kappa_l$ calculated from $(11)_1$ via the PWE and MM formulas by $\mathbf{\Gamma}[N]_{\text{PWE}}$ and $\mathbf{\Gamma}[N]_{\text{MM}}$, respectively. By analogy with [22], it can be proved that

$$\begin{aligned} N_1 \leq N_2 \ &\Rightarrow \mathbf{\Gamma}[N_1]_{\text{MM}} \geq \mathbf{\Gamma}[N_2]_{\text{MM}}\,,\ \mathbf{\Gamma}[N_1]_{\text{PWE}} \geq \mathbf{\Gamma}[N_2]_{\text{PWE}}\,; \\ \forall N \ &\Rightarrow \mathbf{\Gamma} \leq \mathbf{\Gamma}[N]_{\text{MM}} \leq \mathbf{\Gamma}[N]_{\text{PWE}}\,, \end{aligned} \tag{64}$$

where the inequality sign between two matrices is understood in the sense that their difference is a sign definite matrix and hence the differences of their similarly ordered eigenvalues are sign definite. The inequalities $(64)_1$ imply that the MM and PWE approximations of $\mathbf{\Gamma}$ obtained by truncating Eq. $(11)_1$ are upper bounds which converge from above to the exact value with growing N. Furthermore, the MM approximation of $\mathbf{\Gamma}$ is more accurate than the PWE one at a given N, from $(64)_2$.

Taking $N = 0$ in $(64)_2$ yields

$$\mathbf{\Gamma} \leq \mathbf{\Gamma}[0]_{\text{MM}} \leq \mathbf{\Gamma}[0]_{\text{PWE}} = \langle \mathbf{\Gamma} \rangle\,, \tag{65}$$

where $\mathbf{\Gamma}[0]_{\text{MM}}$ admits an explicit expression which is however rather cumbersome. Seeking a simpler result, consider the above inequalities for one of the principal directions $\kappa \parallel \mathbf{e}_l$ so that $\mathbf{\Gamma}(\kappa) = \mathbf{C}_{ll}^{\text{eff}}$. Denote the PWE and MM approximations (15) and (28) of $\mathbf{C}_{ll}^{\text{eff}}$ by $\mathbf{C}_{ll}^{\text{eff}}[N]_{\text{PWE}}$ and $\mathbf{C}_{ll}^{\text{eff}}[N]_{\text{MM}}$. From (65),

$$\mathbf{C}_{ll}^{\text{eff}} \leq \mathbf{C}_{ll}^{\text{eff}}[0]_{\text{MM}} \leq \mathbf{C}_{ll}^{\text{eff}}[0]_{\text{PWE}} = \langle \mathbf{C}_{ll} \rangle\,, \tag{66}$$

where $\mathbf{C}_{ll}^{\text{eff}}\,[0]_{\text{MM}}$ admits closed-form expression as follows. From (27d) and (27e) taken with $N=0$ (i.e. with $\mathbf{g},\mathbf{g}'=\mathbf{0}$),

$$\mathbf{Q}_0\,[0]=\begin{pmatrix}\mathbf{0} & \langle\mathbf{C}_{ll}\rangle_{\bar{l}}^{-1}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}\ \Rightarrow\ \mathbf{M}_0(1)=\begin{pmatrix}\mathbf{I}_3 & \langle\langle\mathbf{C}_{ll}\rangle_{\bar{l}}^{-1}\rangle_l\\ \mathbf{0} & \mathbf{I}_3\end{pmatrix}, \tag{67}$$

so that (28) with $N=0$ yields

$$\mathbf{C}_{ll}^{\text{eff}}[0]_{\text{MM}}=\begin{pmatrix}\mathbf{0} & \mathbf{I}_3\end{pmatrix}\mathbf{S}[0]\equiv\mathbf{S}_2\quad\text{with}\ \ \mathbf{S}[0]=\begin{pmatrix}\mathbf{0} & \langle\langle\mathbf{C}_{ll}\rangle_{\bar{l}}^{-1}\rangle_l\\ \mathbf{0} & \mathbf{0}\end{pmatrix}^{-1}\begin{pmatrix}\mathbf{I}_3\\ \mathbf{0}\end{pmatrix}\equiv\begin{pmatrix}\mathbf{S}_1\\ \mathbf{S}_2\end{pmatrix}. \tag{68}$$

Solving for $\mathbf{S}_2$ gives

$$\begin{pmatrix}\mathbf{0} & \langle\langle\mathbf{C}_{ll}\rangle_{\bar{l}}^{-1}\rangle_l\\ \mathbf{0} & \mathbf{0}\end{pmatrix}\begin{pmatrix}\mathbf{S}_1\\ \mathbf{S}_2\end{pmatrix}=\begin{pmatrix}\mathbf{I}_3\\ \mathbf{0}\end{pmatrix}\ \Rightarrow\mathbf{S}_2=\langle\langle\mathbf{C}_{ll}\rangle_{\bar{l}}^{-1}\rangle_l^{-1}. \tag{69}$$

Thus from (66), (68) and (69),

$$\mathbf{C}_{ll}^{\text{eff}}\le\langle\langle\mathbf{C}_{ll}\rangle_{\bar{l}}^{-1}\rangle_l^{-1}\le\langle\mathbf{C}_{ll}\rangle \tag{70}$$

where $\langle\mathbf{C}_{ll}\rangle$ is identifiable as the Voigt average [17], known to provide an upper bound. The upper bound provided by the first inequality in (70) has not to our knowledge been presented before.

Combining the new bound from (70) with the Voigt inequality $\mathbf{C}_{al}^{\text{eff}}\le\langle\mathbf{C}_{al}\rangle$ $(a\neq l)$ yields

$$\mathbf{\Gamma}(\kappa)\le\mathbf{\Gamma}_{\text{B}}(\kappa)\equiv\left(\langle\mathbf{C}_{al}\rangle\kappa_a\kappa_l\right)_{a\neq l}+\langle\langle\mathbf{C}_{ll}\rangle_{\bar{l}}^{-1}\rangle_l^{-1}\kappa_l^2, \tag{71}$$

where the subscript "B" implies bound. Denote the eigenvalues of the matrix $\mathbf{\Gamma}_{\text{B}}$ by $\langle\rho\rangle\,c_{\text{B}\alpha}^2$ and order them in the same way as the eigenvalues $\langle\rho\rangle\,c_\alpha^2$ of $\mathbf{\Gamma}$, then it follows that

$$c_\alpha(\kappa)\le c_{\text{B}\alpha}(\kappa),\ \ \alpha=1,2,3. \tag{72}$$

It will be demonstrated in §5 that the upper bounds $c_{\text{B}\alpha}$ of the effective speeds can also serve as their reasonable estimate.

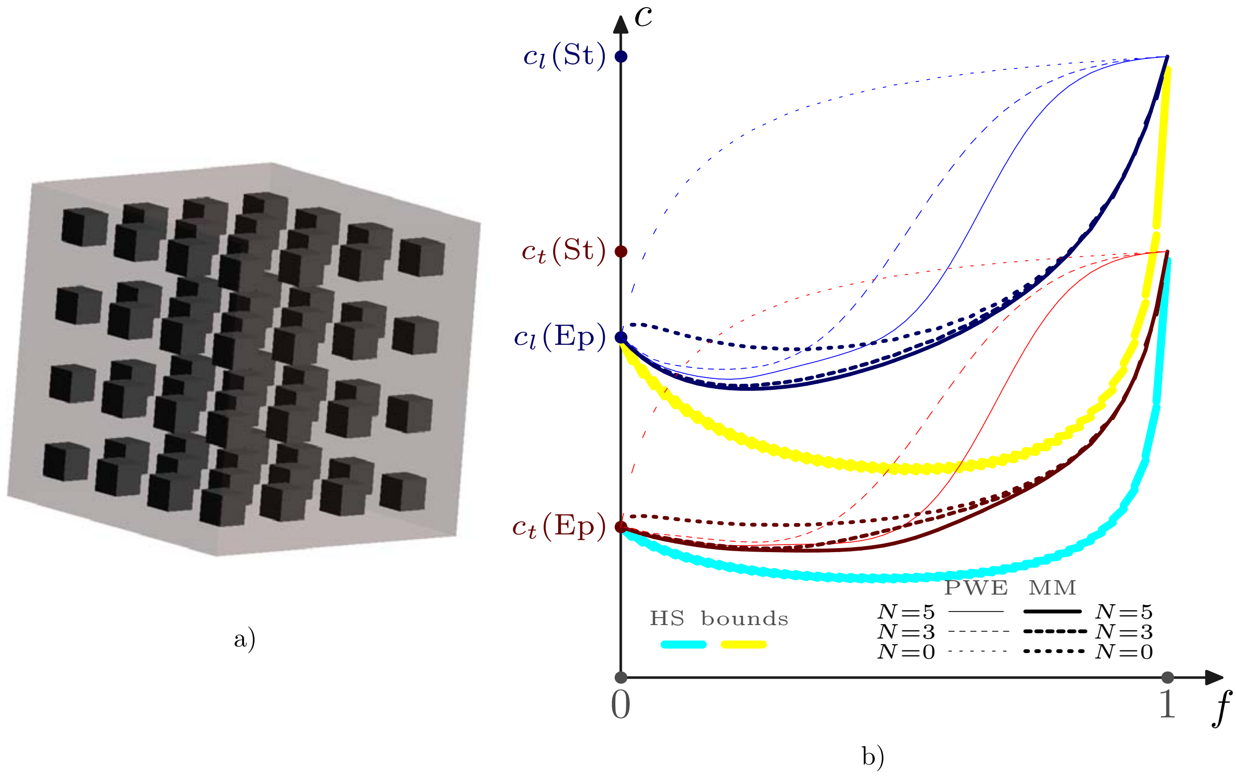

Figure 1: (a) A cubic lattice of symmetric steel cubes in Epoxy at filling fraction $f = 1/8$. (b) Effective wave speeds as a function of f. The PWE and MM calculated values are plotted by thin and thick lines (light blue and red online), respectively. The broad curves indicate the Hashin-Shtrikman lower bounds.

5. Numerical examples

We consider two examples of 3D phononic crystals composed of steel inclusions in epoxy matrix. The material parameters are c_{11} (St) = 170 GPa, c_{66} (St) = 80 GPa, ρ (St) = 7.7 g/cm^3 for steel and c_{11} (Ep) = 7.537 GPa, c_{66} (Ep) = 1.482 GPa, ρ (Ep) = 1.142 g/cm^3 for epoxy. This implies c_l (St) = 4.7 mm/μs, c_t (St) = 3.22 mm/μs and c_l (Ep) = 2.57 mm/μs, c_t (Ep) = 1.14 mm/μs for the longitudinal and transverse speeds. The number of Fourier modes is $(2N+1)^3$ for the PWE method and $(2N+1)^2$ for the MM method; we performed the calculations for $N = 0, 3, 5$.

The first example assumes a cubic lattice of cubic steel inclusions (Fig. 1a). We present the effective longitudinal and transverse speeds c_l and c_t in the principal direction as functions of the volume fraction of steel inclusions (Fig. 1b). The curves calculated by the PWE method are plotted by thin lines (light blue and red online), the curves calculated by the MM method are plotted by thick lines (dark blue and red online). For each method, we present three different data obtained with $N = 0$, $N = 3$ and $N = 5$ (dotted, dashed and solid lines, respectively). The Hashin-Shtrikman lower bounds [23] are also plotted (the Hashin-Shtrikman upper bounds lie far above the other curves and are not displayed). It is observed from Fig. 1b that the results of both methods monotonically converge from above to the exact value with growing N in agreement with the general statement of §4. What is significant is that the convergence of the MM method is seen to be much faster than that of the PWE method. In fact, the explicit MM estimate for $N = 0$ which follows from (70) in the form

$$c_l^2 = \frac{1}{\langle\rho\rangle}\left\langle\langle c_{11}\rangle_{\bar{1}}^{-1}\right\rangle_1^{-1},\ c_t^2 = \frac{1}{\langle\rho\rangle}\left\langle\langle c_{66}\rangle_{\bar{1}}^{-1}\right\rangle_1^{-1}, \tag{73}$$

provides a much better estimate for c_l and c_t at $f > 0.5$ than the PWE calculation with $N = 5$, i.e. with matrices of about 4000×4000 size. Note that as $f \to 1$ in the example of Fig. 1, the bound (70) may be approximated, yielding

$$c_{11}^{\text{eff}} \lessapprox \Big(\frac{1}{c_{11}(\text{St})} + \frac{1 - f^{1/3}}{c_{11}(\text{Ep})} \Big)^{-1}. \tag{74}$$

At the same time the geometry of the unit cell for $f \to 1$ indicates that the modulus c_{11}^{eff} can be estimated by an equivalent medium stratified in the 1−direction, for which the uniaxial strain assumption with constant stress σ_{11} leads to the approximation $c_{11}^{\text{eff}} \approx \langle c_{11}^{-1} \rangle^{-1}$, the same as the right hand side of (74) (as $f \to 1$). This, combined with the fact that $1 - f^{1/3}$ tends to zero faster than $1 - f$ as $f \to 1$, explains the exceptional accuracy of the new bound as an estimate for the moduli. Note that, by comparison, the Hashin-Shtrikman bounds (upper or lower) do not provide a useful estimate in this case.

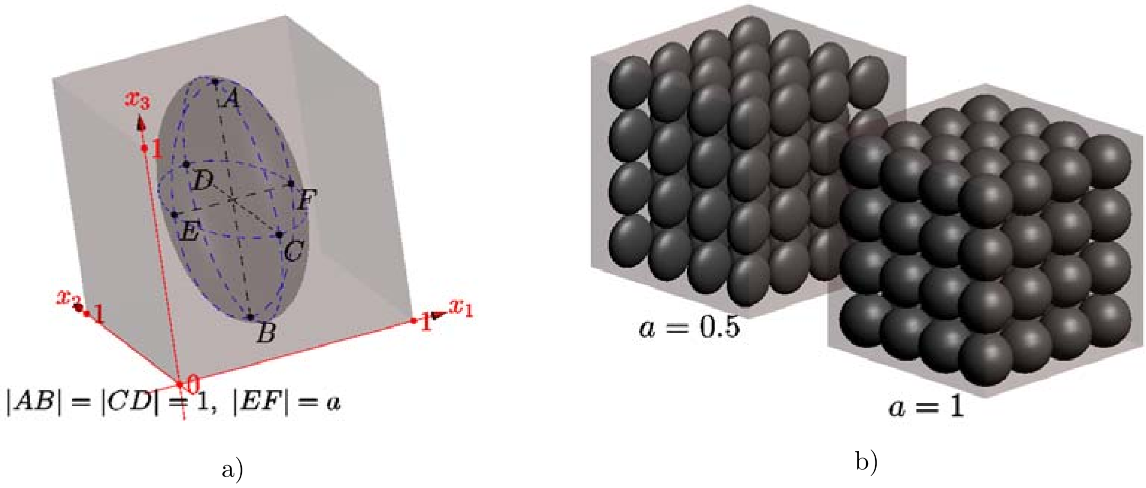

Figure 2: A cubic lattice of Steel spheroids in Epoxy matrix. (a) The inclusions are oblate spheroids with minor axis a and unit major axes. (b) The periodic structure for $a = 0.5$ and $a = 1$ (spheres).

The second example considers a cubic lattice of spheroidal steel inclusions in epoxy matrix. The shape of the inclusion evolves from formally a disk of unit diameter to a ball of unit diameter (that is, inscribed in a cubic unit cell) by means of elongating the radius along the x_1 direction, see Fig. 2. We describe the dependence of the effective speeds c_l and c_t along x_1 and of the corresponding effective elastic moduli c_{11} and c_{66} on the shape of the spheroidal inclusion. Fourier coefficients for the PWE and MM methods are given in Appendix 2. The results are obtained by the PWE method with $N = 3$ and $N = 5$ (open circles in Fig. 3) and by the MM method with $N = 0$, $N = 3$ and $N = 5$ (dotted, dashed and solid lines in Fig. 3). The MM method is particularly efficient for the case in hand since it uses Fourier coefficients in the x_2x_3 plane where the inclusions have circular cross-section and performs direct numerical integration of the Riccati equation (see §3.2) along the direction x_1 where the shape is 'distorted'. We observe an interesting feature of a drastic increase of the effective longitudinal speed c_l and of the modulus c_{11} when the inclusions tend to touch each other, see Fig. 3a. This type of configuration where the inclusions are almost touching is known to be particularly difficult for numerical calculation of the effective properties [10]. MM appears to be particularly well suited to treating such problems with closely spaced inclusions since it explicitly accounts for the thin gap region via integration of the Riccati equation. The PWE method, on the other hand, clearly fails to capture the sharp increase in wave speed at $N = 5$ (matrix size $\approx 4000 \times 4000$). In fact, the PWE for $N = 3$ does not even satisfy the strict upper bounds (73) derived from MM at $N = 0$.

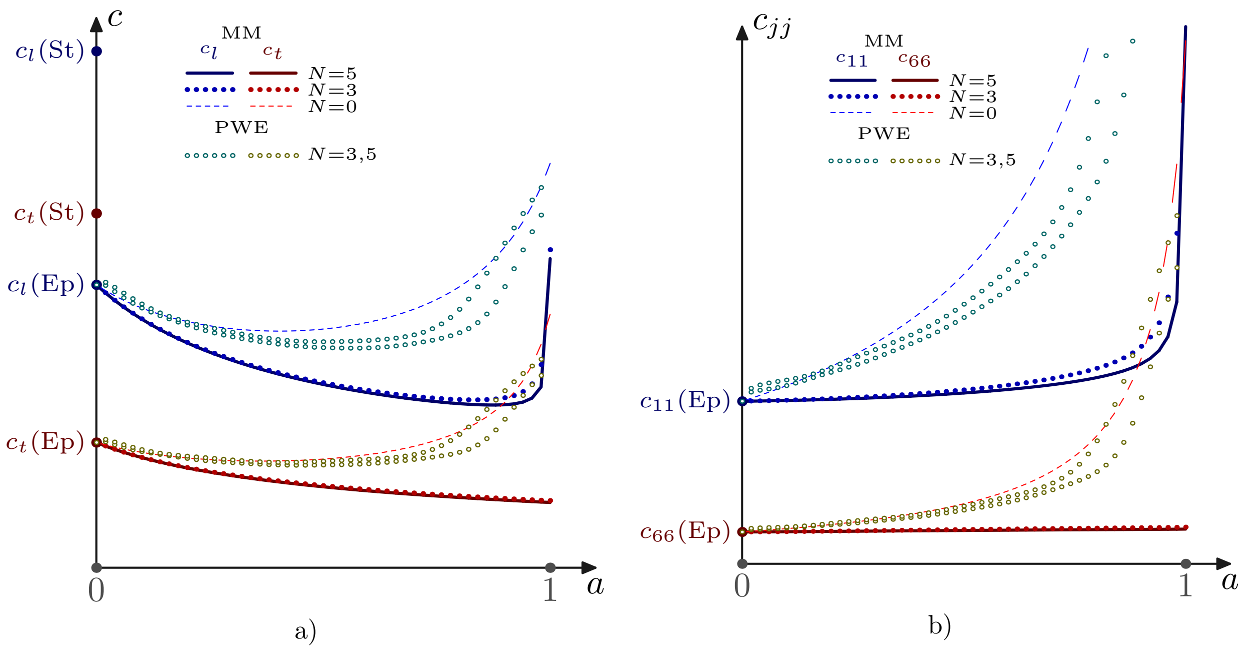

Figure 3: (a) Effective wave speeds for the periodic structure of Fig. 2 as a function of the spheroid minor axis a calculated by the PWE and MM methods. (b) The corresponding elastic moduli.

6. Conclusion

The PWE and MM methods of calculating quasistatic effective speeds in three-dimensional phononic crystals have been formulated and compared. The MM method can be viewed as a two-dimensional PWE combined with a one-dimensional propagator matrix approach. The propagator part of the MM scheme is calculated by numerical integration of a (nonlinear) Riccati differential equation to produce the monodromy matrix.

It was shown both analytically and numerically that the MM method provides more accurate approximations than the PWE scheme. In particular, the closed form MM bounds (70) (see also (73)) using only one Fourier mode to estimate the effective speed gives better approximations than PWE bounds using more than a thousand (eleven in each of x_i, $i = 1, 2, 3$) Fourier modes in the case of densely packed structures (see Fig. 1b for $f > 0.5$).

The speed-up of the MM method as compared with PWE via reduction in matrix size is particularly significant for the three-dimensional homogenization problem. Thus, numerical implementation of the PWE scheme needs a matrix of dimension $3(2N+1)^3 \times 3(2N+1)^3$, requiring a considerable amount of computer memory even for small N. By contrast, the MM scheme uses matrices of dimension $6(2N+1)^2 \times 6(2N+1)^2$. The reduced memory requirement for the MM method is at the cost of the computer time needed to solve the Riccati equation, a relatively small price to pay. In fact, the ability to set the step size in the Runge-Kutta scheme enables the MM method to efficiently and accurately solve configurations for which the PWE is particularly ill-suited, such as narrow gaps (see Fig. 1b for $f \to 1$) and closely spaced inclusions (Fig. 3 for $a \to 1$).

Appendix

Appendix 1. Alternative derivation of Eq. (25) for $\mathbf{C}_{ll}^{\text{eff}}$.

Let $\mathbf{k}$ be parallel to one of the translation vectors. Take the latter to be $\mathbf{e}_1 = (\delta_{1i})$ and so $\mathbf{k} = (k_1, 0, 0)$. Equation (3) may be rewritten in the form

$$\boldsymbol{\eta}' = (\boldsymbol{\mathcal{Q}}_0 + \omega^2 \boldsymbol{\mathcal{Q}}_1)\boldsymbol{\eta} \quad \text{where } ' \equiv \partial_1, \quad \boldsymbol{\eta} = \begin{pmatrix} \mathbf{v} \\ \mathbf{C}_{1p}\partial_p \mathbf{v} \end{pmatrix}, \; \boldsymbol{\mathcal{Q}}_1 = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ -\rho \mathbf{I}_3 & \mathbf{0} \end{pmatrix}, \tag{75}$$

while $\boldsymbol{\mathcal{Q}}_0$ is defined in (18) and (19) with $j = 1$ and $a, b = 2, 3$. Denote $\boldsymbol{\eta}(x_1) \equiv \boldsymbol{\eta}(x_1, x_2, x_3)$. The solution to (75) with some initial function $\boldsymbol{\eta}(0)$ can be written via the matricant in the form

$$\boldsymbol{\eta}(x_1) = \boldsymbol{\mathcal{M}}(x_1)\boldsymbol{\eta}(0) \quad \text{with } \boldsymbol{\mathcal{M}}(x_1) = \widehat{\int_0^{x_1}} (\boldsymbol{\mathcal{I}} + (\boldsymbol{\mathcal{Q}}_0 + \omega^2 \boldsymbol{\mathcal{Q}}_1) dx_1). \tag{76}$$

Taking into account assumed 1-periodicity in x_1 and hence the Floquet condition $\mathbf{v} = e^{ik_1 x_1}\mathbf{u}$ for the solution of (3) implies that the solution $\boldsymbol{\eta}$ of (75) must satisfy $\boldsymbol{\eta}(1) = e^{ik_1}\boldsymbol{\eta}(0)$. Thus, with reference to (76), $\omega(k_1, 0, 0) \equiv \omega(k_1)$ is an eigenvalue of (3) iff there exists $\mathbf{w} \equiv \mathbf{w}(x_2, x_3)$ such that

$$\boldsymbol{\mathcal{M}}(1)\mathbf{w} = e^{ik_1}\mathbf{w}. \tag{77}$$

Consider asymptotic expansion of (77) in small ω, k_1. By (76),

$$\begin{gathered} \boldsymbol{\mathcal{M}}(1) = \boldsymbol{\mathcal{M}}_0 + \omega^2 \boldsymbol{\mathcal{M}}_1 + O(\omega^4) \quad \text{where} \\ \boldsymbol{\mathcal{M}}_0 \equiv \boldsymbol{\mathcal{M}}_0[1, 0], \quad \boldsymbol{\mathcal{M}}_0[b, a] = \widehat{\int_a^b} (\boldsymbol{\mathcal{I}} + \boldsymbol{\mathcal{Q}}_0 \mathrm{d}x_1), \quad \boldsymbol{\mathcal{M}}_1 = \int_0^1 \boldsymbol{\mathcal{M}}_0[1, x_1]\, \boldsymbol{\mathcal{Q}}_1 \boldsymbol{\mathcal{M}}_0[x_1, 0]\, \mathrm{d}x_1. \end{gathered} \tag{78}$$

The identity $\boldsymbol{\mathcal{M}}_0 \mathbf{W}_0 = \mathbf{W}_0$ with the 6×3 matrix $\mathbf{W}_0 = (\mathbf{I}_3 \; \mathbf{0})^+$ (see (21)) implies triple multiplicity of the zero-order $\omega = 0$. Therefore we may write

$$\omega_\alpha(k_1) = c_\alpha k_1 + O(k_1^2), \quad \mathbf{w}_\alpha = \mathbf{w}_{0\alpha} + k_1 \mathbf{w}_{1\alpha} + k_1^2 \mathbf{w}_{2\alpha} + \mathbf{O}(k_1^3) \text{ with } \mathbf{w}_{0\alpha} = \mathbf{W}_0 \mathbf{u}_{0\alpha}, \tag{79}$$

where $\alpha = 1, 2, 3$ and $\mathbf{u}_{0\alpha}$ are some constant linear independent 3×1 vectors. Inserting (78)-(79) along with $e^{ik_1} = 1 + ik_1 - \frac{1}{2}k_1^2 + O(k_1^3)$ in (77) and equating the terms of the same order in k_1 yields

$$1: \boldsymbol{\mathcal{M}}_0 \mathbf{w}_{0\alpha} = \mathbf{w}_{0\alpha}, \tag{80a}$$

$$k_1: \boldsymbol{\mathcal{M}}_0 \mathbf{w}_{1\alpha} = i\mathbf{w}_{0\alpha} + \mathbf{w}_{1\alpha}, \tag{80b}$$

$$k_1^2: \boldsymbol{\mathcal{M}}_0 \mathbf{w}_{2\alpha} + c_\alpha^2 \boldsymbol{\mathcal{M}}_1 \mathbf{w}_{0\alpha} = -\frac{1}{2}\mathbf{w}_{0\alpha} + i\mathbf{w}_{1\alpha} + \mathbf{w}_{2\alpha}. \tag{80c}$$

Express $\mathbf{w}_{1\alpha}$ from (80b) and substitute it in (80c), then scalar multiply the latter by the 6×3 matrix $\widetilde{\mathbf{W}}_0 = (\mathbf{0} \; \mathbf{I}_3)^+$ satisfying the identity $\boldsymbol{\mathcal{M}}_0^+[b, a]\, \widetilde{\mathbf{W}}_0 = \widetilde{\mathbf{W}}_0$ (see (21)). As a result, we obtain

$$\mathbf{C}_{11}^{\text{eff}} = \langle \widetilde{\mathbf{W}}_0^+ (\boldsymbol{\mathcal{M}}_0 - \boldsymbol{\mathcal{I}})^{-1} \mathbf{W}_0 \rangle_{\bar{1}} \quad \text{for } \kappa = \mathbf{e}_1 = (\delta_{1i}). \tag{81}$$

It is seen that (25) with $\boldsymbol{\mathcal{M}}_0(1) \equiv \boldsymbol{\mathcal{M}}_0$ and $l = 1$ is the same as (81), QED.

Appendix 2. Fourier coefficients for spheroidal inclusions

The coefficients for the spheroids of Fig. 2a are as follows:

1. MM method. Identity (27) yields

$$\widehat{\mathbf{C}}_{pq}(g_2, g_3, x_1) = \begin{cases} \mathbf{C}_{pq}(\text{Ep}), & x_1 \notin \left[\frac{1-a}{2}, \frac{1+a}{2}\right], \\ \mathbf{C}_{pq}(\text{Ep}) + (\mathbf{C}_{pq}(\text{St}) - \mathbf{C}_{pq}(\text{Ep}))\hat{\chi}_1(g_2, g_3, x_1), & x_1 \in \left[\frac{1-a}{2}, \frac{1+a}{2}\right] \end{cases}$$

with

$$\hat{\chi}_1(g_2, g_3, x_1) = (-1)^{g_2+g_3} \frac{RJ_1(2\pi R\sqrt{g_2^2+g_3^2})}{\sqrt{g_2^2+g_3^2}}, \quad R^2 = 1 - \frac{(2x_1-1)^2}{a^2},$$

where J_1 is the first order Bessel function.

2. PWE method. Identity (13) yields

$$\widehat{\mathbf{C}}_{pq}(\mathbf{g}) = \mathbf{C}_{pq}(\text{Ep})\delta_{\mathbf{g0}} + (\mathbf{C}_{pq}(\text{St}) - \mathbf{C}_{pq}(\text{Ep}))\hat{\chi}_2(\mathbf{g}),$$

where

$$\hat{\chi}_2(\mathbf{g}) = \frac{a(-1)^{g_1+g_2+g_3}}{2\pi^2|\mathbf{g}_a|^3}(\sin(\pi|\mathbf{g}_a|) - \pi|\mathbf{g}_a|\cos(\pi|\mathbf{g}_a|)), \quad |\mathbf{g}_a| = \sqrt{(ag_1)^2 + g_2^2 + g_3^2}$$

and δ is a Kronecker symbol.

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