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Effective Willis constitutive equations for periodically stratified anisotropic elastic media

A.L. Shuvalov^a, A.A. Kutsenko^a, A.N. Norris^{a,b}, O. Poncelet^a

^a Université de Bordeaux, CNRS, UMR 5469,
Laboratoire de Mécanique Physique, Talence 33405, France

^b Mechanical and Aerospace Engineering, Rutgers University,
Piscataway, NJ 08854-8058, USA

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Abstract

A method to derive homogeneous effective constitutive equations for periodically layered elastic media is proposed. The crucial and novel idea underlying the procedure is that the coefficients of the dynamic effective medium can be associated with the matrix logarithm of the propagator over a unit period. The effective homogeneous equations are shown to have the structure of a Willis material, characterized by anisotropic inertia and coupling between momentum and strain, in addition to effective elastic constants. Expressions are presented for the Willis material parameters which are formally valid at any frequency and horizontal wavenumber as long as the matrix logarithm is well defined. The general theory is exemplified for scalar SH motion. Low frequency, long wavelength expansions of the effective material parameters are also developed using a Magnus series and explicit estimates for the rate of convergence are derived.

1 Introduction

Elastic waves in periodically layered or continuous (functionally graded) elastic media of general anisotropy have been studied extensively by different methods. Among them is the sextic formalism of Stroh, which incorporates the elastodynamics equations into a first-order ordinary differential equation for the displacement-traction state vector with system matrix \mathbf{Q} composed of material parameters [1]. The wave-field propagator matrix along the stratification direction y , $\mathbf{M}(y, 0)$, is given by the Peano series of multiple integrals of products of $\mathbf{Q}(y)$ [2]. This is essentially a power series in distance-to-wavelength ratio, which is therefore particularly well-suited to tackling the problem of approximating a periodically stratified medium by an effective homogeneous medium. The Stroh formalism clarifies the meaning of zero-order homogenization, or static averaging, of a periodic medium by revealing the zero-order effective material parameters [3, 4] as nothing more than the matrix $\mathbf{Q}(y)$ integrated over the period T , which is the leading term of the logarithm of the Peano series for $\mathbf{M}(T, 0)$ [5]. Static averaging implies a non-dispersive effective medium. Generalization to a higher-order effective homogeneous medium, which must be dispersive, is less obvious. Its derivation is commonly based on the long-wave dispersion of the fundamental Bloch or Floquet branches. Their onset in arbitrary anisotropic periodically stratified media was analyzed in [5]; on this basis, the scalar-wave equation for a transversely isotropic dispersive effective medium

was modelled in [5, 6, 7] and in the subsequent literature (see e.g. [8] and its bibliography). A semi-analytical approach for general anisotropy [9] (see also [10]) fits the long-wave Floquet dispersion to statically averaged effective constants, such that the effective medium is seen as a "continuum of non-dispersive media" that are different for different frequency and propagation direction.

In this paper a new method is proposed for finding dynamic effective constitutive equations at finite frequencies and wavelength. This is achieved by explicit construction of effective spatially constant material coefficients that reproduce exactly the monodromy matrix $\mathbf{M}(T, 0)$. The effective constitutive theory is exact in the sense that it give the correct displacement-traction field at the unit-cell interfaces over arbitrary long distance of propagation. Two key steps distinguish the method advocated. First is the idea, based on the Floquet theorem, of defining the effective medium such that the sextic system of elastodynamics equations in this medium has the matrix of coefficients \mathbf{Q}_{eff} equal to $i\mathbf{K}$, where \mathbf{K} is the Floquet wave number matrix with an exact definition $i\mathbf{K}T = \ln \mathbf{M}(T, 0)$. For the low-frequency long-wave range, a matrix logarithm $\ln \mathbf{M}(T, 0)$ admits an expansion called the Magnus series [11]. Restricting it to the leading-order term leads to the statically averaged effective model (see above). Taking the next-order term(s) of the Magnus expansion for \mathbf{K} reveals that, unless the variation of material properties over a period is symmetric, the above-defined dispersive effective medium cannot be fitted to the standard form of elastodynamic equations, in which the frequency dispersion and non-locality would be fully accounted by the dependence of effective density and elasticity on ω and k_x . This motivates the second significant step in the present method which is identifying a class of constitutive models that does fit $i\mathbf{K}$ with the system matrix \mathbf{Q}_{eff} of a homogeneous medium. We demonstrate by construction that the model described by the Willis constitutive relations with a dynamic stress-impulse coupling tensor [13, 14] provides such a class of materials. Expansions of the Willis material coefficients based on the Magnus series for \mathbf{K} are obtained in the low-frequency long-wave range where they are analytic in ω , k_x . Explicit estimates of the dependence on ω , k_x are found that enable closed-form asymptotics of the Willis coefficients with a desired accuracy. At the same time, the definition $i\mathbf{K}T = \ln \mathbf{M}(T, 0)$ and the fitting of the matrix $\mathbf{Q}_{\text{eff}} \equiv i\mathbf{K}$ to the effective Willis material is formally not restricted to the low-frequency long-wave range.

A significant outcome of the proposed approach is that fairly explicit expressions are obtained for the effective material parameters. This is particularly evident for the example of SH (shear horizontal) waves discussed in detail in §4. In this regard the approach is distinct from that of [14] which leads to expressions for the parameters in the (spatial) transform domain. Note also that the results here apply to a single realization of the layered medium, no ensemble averaging is invoked. This point is discussed further in §4.

The paper proceeds as follows. The problem is formulated in §2 where the sextic formalism for periodically stratified media is outlined, the Floquet wave number matrix \mathbf{K} introduced and its Magnus expansion examined (see also Appendix A). The main results of the paper are derived in §3. It starts by observing that the matrix $i\mathbf{K}$ viewed as a sextic-system matrix \mathbf{Q}_{eff} for a homogeneous effective medium cannot be associated with a medium from the class of anisotropic elastic materials but it does fit the Willis model. Using the *ansatz* that the sought effective medium is described by the spatially homogeneous equations for a Willis material, the corresponding system matrix \mathbf{Q}_{eff} is constructed and equated with $i\mathbf{K}$. Under certain assumptions, a prescription for unique definition of the Willis effective medium is put forward. The remainder of §3 discusses general properties of the Willis material parameters. The example of SH wave motion in a periodic structure is considered in §4. It illustrates the method for defining effective coefficients of the Willis model beyond the Magnus series expansion (which in its turn is detailed for SH waves in Appendix B). The obtained explicit expressions are used to solve a reflection-transmission problem at the interface of the effective medium. Conclusions are presented in §5.

2 Background

2.1 Stroh formalism and the wave number matrix \mathbf{K}

We consider a Cartesian elastic medium with density $\rho = \rho(y)$ and stiffness tensor $c_{ijkl} = c_{ijkl}(y)$. Basic notations used include the superscripts T , $+$ and $*$ for transposition, Hermitian and complex conjugation, respectively, and \mathbf{T} for the matrix with zero diagonal and identity off-diagonal blocks.

Taking the Fourier transforms of the equilibrium and stress-strain equations

$$\sigma_{ij,i} = \rho \ddot{u}_j, \quad \sigma_{ij} = c_{ijkl} e_{kl}, \quad (1)$$

in all variables except y leads to an ordinary differential problem for the quasi-plane modes with the phase factor $e^{i(k_x x - \omega t)}$, where ω is the frequency and k_x the wavenumber in an arbitrary chosen direction X orthogonal to Y (rotating X causes all 21 elastic constants c_{ijkl} to appear). Denote the unit vectors parallel to X and Y by \mathbf{m} and \mathbf{n} so that $x = \mathbf{m} \cdot \mathbf{r}$, $y = \mathbf{n} \cdot \mathbf{r}$, and let $\mathbf{A}(y)$ and $\mathbf{F}(y)$ be the amplitudes of displacement \mathbf{u} and traction $\mathbf{n}\sigma$, respectively. Then Eqs. (1) combine into the Stroh system

$$\frac{d}{dy} \eta(y) = \mathbf{Q}(y) \eta(y) \quad (2)$$

for the state vector η incorporating \mathbf{A} and \mathbf{F} [1]. Taking it in the form $\eta = (\mathbf{A}, i\mathbf{F})^{\text{T}}$ defines the 6×6 system matrix as

$$\mathbf{Q}(y) = i \begin{pmatrix} k_x \mathbf{N}_1 & \mathbf{N}_2 \\ k_x^2 \mathbf{N}_3 - \rho \omega^2 \mathbf{I} & k_x \mathbf{N}_1^{\text{T}} \end{pmatrix} \quad (3)$$

via the 3×3 blocks \mathbf{N}_J of the Stroh matrix

$$\mathbf{N}(y) = \begin{pmatrix} \mathbf{N}_1 & \mathbf{N}_2 \\ \mathbf{N}_3 & \mathbf{N}_1^{\text{T}} \end{pmatrix}, \quad \mathbf{N}_1 = - (nn)^{-1} (nm) = \mathbf{N}_4^{\text{T}}, \quad \mathbf{N}_2 = - (nn)^{-1}, \quad (4)$$

$$\mathbf{N}_3 = (mm) - (mn) (nn)^{-1} (nm),$$

which is composed of the matrices with elements $(nn)_{jk} = n_i c_{ijkl} m_l$, $(nm)_{jk} = n_i c_{ijkl} m_l = (mn)_{kj}$ and $(mm)_{jk} = m_i c_{ijkl} m_l$ (note that \mathbf{N}_2 is negative definite). The usual indicial symmetry of c_{ijkl} used in (4) leads to a Hamiltonian structure $\mathbf{N} = \mathbf{T} \mathbf{N}^{\text{T}} \mathbf{T}$ and $\mathbf{Q} = \mathbf{T} \mathbf{Q}^{\text{T}} \mathbf{T}$ of \mathbf{N} and \mathbf{Q} . Since ω , k_x and ρ , c_{ijkl} are real and hence $\mathbf{Q}(y)$ is imaginary, it follows that $\mathbf{Q} = -\mathbf{T} \mathbf{Q}^+ \mathbf{T}$. The latter identity on its own suffices to ensure energy conservation. Alternative definitions of η and hence of \mathbf{Q} may be chosen. In general, the eigenvalues of $\mathbf{Q}(y)$ are first-degree homogeneous functions of ω , k_x , which implies absence of dispersion.

Given the initial condition at some $y_0 (\equiv 0)$, the solution to (2) is $\eta(y) = \mathbf{M}(y, 0) \eta(0)$, where $\mathbf{M}(y, 0)$ is the 6×6 matricant evaluated by the Peano series [2]

$$\mathbf{M}(y, 0) = \mathbf{I} + \int_0^y \mathbf{Q}(y_1) dy_1 + \int_0^y \mathbf{Q}(y_1) dy_1 \int_0^{y_1} \mathbf{Q}(y_2) dy_2 + \int_0^y \int_0^{y_1} \int_0^{y_2} \dots \quad (5)$$

Suppose now that ρ , c_{ijkl} and hence \mathbf{Q} depend on y periodically with a period T . Denote

$$y = \tilde{y} + nT, \quad \tilde{y} = y \bmod T \in [0, T], \quad \tilde{\zeta} = \frac{\tilde{y}}{T} \in [0, 1], \quad \langle \cdot \rangle = \frac{1}{T} \int_0^T \cdot d\tilde{y} = \int_0^1 \cdot d\tilde{\zeta}, \quad (6)$$

where $\langle \dots \rangle$ is the static average over a unit cell. It is understood hereafter that the wave-path distance y includes a large enough number n of periods, which is when the present development is of interest. By (5), the matricant $\mathbf{M}(T, 0)$ over $[0, T]$, which is called the monodromy matrix, is

$$\mathbf{M}(T, 0) = \mathbf{I} + \sum_{m=1}^{\infty} \mathbf{M}^{(m)} = \mathbf{I} + T \langle \mathbf{Q} \rangle + T^2 \int_0^1 \mathbf{Q}(\tilde{\zeta}) d\tilde{\zeta} \int_0^{\tilde{\zeta}} \mathbf{Q}(\tilde{\zeta}_1) d\tilde{\zeta}_1 + \dots \quad (7)$$

The wave number matrix \mathbf{K} is introduced by denoting the monodromy matrix as

$$\mathbf{M}(T, 0) = \exp(i\mathbf{K}T) \Leftrightarrow i\mathbf{K}T = \ln \mathbf{M}(T, 0). \quad (8)$$

In the following, unless otherwise specified, \mathbf{K} is understood as defined in the first Brillouin zone, which implies the zeroth Riemann sheet of $\ln z$ with a cut $\arg z = \pm\pi$. Using (8), the matricant $\mathbf{M}(y, 0)$ can be written as

$$\mathbf{M}(y, 0) = \mathbf{M}(\tilde{y}, 0) \mathbf{M}(nT, 0) = \mathbf{L}(\tilde{y}) \exp(i\mathbf{K}y), \quad (9)$$

where $\mathbf{L}(\tilde{y}) = \mathbf{M}(\tilde{y}, 0) \exp(-i\mathbf{K}\tilde{y})$ with $\mathbf{L}(0) = \mathbf{L}(T) = \mathbf{I}$. Eq. (9)₂ represents the Floquet theorem. Denote the eigenvalues of $\mathbf{M}(T, 0)$ and \mathbf{K} by $e^{iK_\alpha T}$ and K_α ($\alpha = 1..6$), respectively. In the general case where $\mathbf{M}(T, 0)$ and \mathbf{K} have six linear independent eigenvectors \mathbf{w}_α , the Floquet theorem implies that the wave field $\eta(y) = \mathbf{M}(y, 0) \eta(0)$ with the initial data expanded as $\eta(0) = \sum_\alpha C_\alpha \mathbf{w}_\alpha$ takes the form

$$\eta(y) = \sum_{\alpha=1}^6 C_\alpha \eta_\alpha(y) \text{ where } \eta_\alpha(y) = \mathbf{L}(\tilde{y}) \mathbf{w}_\alpha e^{iK_\alpha y}. \quad (10)$$

The identity $\mathbf{Q} = -\mathbf{T}\mathbf{Q}^+\mathbf{T}$ yields $\mathbf{M}^{-1}(y, 0) = \mathbf{T}\mathbf{M}^+(y, 0)\mathbf{T}$, which leads in turn to $\mathbf{L}^{-1}(\tilde{y}) = \mathbf{T}\mathbf{L}^+(\tilde{y})\mathbf{T}$ and

$$\mathbf{K} = \mathbf{T}\mathbf{K}^+\mathbf{T} = \begin{pmatrix} \mathbf{K}_1 & \mathbf{K}_2 \\ \mathbf{K}_3 & \mathbf{K}_1^+ \end{pmatrix} \text{ with } \mathbf{K}_{2,3} = \mathbf{K}_{2,3}^+ \quad (11)$$

for \mathbf{K} defined in the first Brillouin zone. If the unit-cell profile is symmetric, i.e. the variation of material properties within the period T is symmetric about the middle point so that $\mathbf{Q}(\tilde{y})$ is even about $\tilde{y} = T/2$, then the above identities are complemented by $\mathbf{M}(T, 0) = \mathbf{T}\mathbf{M}^T(T, 0)\mathbf{T}$ and hence $\mathbf{K} = \mathbf{T}\mathbf{K}^T\mathbf{T}$; so, with reference to (11), \mathbf{K} is real. Thus

$$\mathbf{K} = \mathbf{T}\mathbf{K}^T\mathbf{T} = \mathbf{K}^* \text{ for a symmetric } \mathbf{Q}(\tilde{y}). \quad (12)$$

2.2 Expansion of \mathbf{K} in the Magnus series

The logarithm of the monodromy matrix $\mathbf{M}(T, 0)$ can be expanded as a Magnus series [11] (see also [12]):

$$\begin{aligned} i\mathbf{K} &= \frac{1}{T} \ln \mathbf{M}(T, 0) = \langle \mathbf{Q} \rangle + \sum_{m=1}^{\infty} i\mathbf{K}^{(m)} \text{ with} \\ i\mathbf{K}^{(1)} &= T \frac{1}{2} \int_0^1 d\tilde{\zeta} \int_0^{\tilde{\zeta}} [\mathbf{Q}(\tilde{\zeta}), \mathbf{Q}(\tilde{\zeta}_1)] d\tilde{\zeta}_1, \\ i\mathbf{K}^{(2)} &= T^2 \frac{1}{6} \int_0^1 d\tilde{\zeta} \int_0^{\tilde{\zeta}} d\tilde{\zeta}_1 \int_0^{\tilde{\zeta}_1} ([\mathbf{Q}, [\mathbf{Q}, \mathbf{Q}]] + [[\mathbf{Q}, \mathbf{Q}], \mathbf{Q}]) d\tilde{\zeta}_2, \text{ etc.}, \end{aligned} \quad (13)$$

where $[\mathbf{Q}(x), \mathbf{Q}(y)] = \mathbf{Q}(x)\mathbf{Q}(y) - \mathbf{Q}(y)\mathbf{Q}(x)$ is a commutator of matrices depending on successive integration variables. Each Magnus series term $\mathbf{K}^{(m)}$ is a $(m+1)$ -tuple integral of permutations of m nested commutators involving products of $(m+1)$ matrices $\mathbf{Q}(\tilde{\zeta}_i)$. A commutator-based form may be anticipated by noting that all $\mathbf{K}^{(m)}$ for $m > 0$ must vanish in the trivial case of a homogeneous material with a constant $\mathbf{Q} \equiv \mathbf{Q}_0$ and hence with $\mathbf{M}(T, 0) = \exp(\mathbf{Q}_0 T)$. For practical calculations it is convenient to use the recursive formulas provided in [11]. In obvious contrast with the Peano expansion, the Magnus series converges in a limited range: the sufficient condition for

its convergence is $\langle \|\mathbf{Q}\|_2 \rangle < \pi/T$, where $\|\cdot\|_2$ is the matrix norm [16]. This condition implies that the eigenvalues $K_\alpha(\omega^2, k_x)$ of \mathbf{K} , defined as continuous functions such that $K_\alpha(0,0) = 0$, satisfy the inequality $\|\text{Re } K_\alpha\| < \pi/T$.

The Magnus series for \mathbf{K} is a low-frequency long-wave expansion. Actually ω and k_x are two independent parameters for \mathbf{Q} and hence for \mathbf{M} and \mathbf{K} . It is however essential that the dependence of 3×3 blocks of \mathbf{Q} on ω and k_x is homogeneous, see (3). Therefore the blocks of each m th term of the Peano and Magnus series are homogeneous polynomials of ω, k_x of degree one greater than the same block of the $(m-1)$ th term. This is what enables introducing a single long-wave parameter $\varepsilon \equiv kT$ with a suitably defined wavenumber k , see (55). Thus the Magnus series (13) is basically an expansion in powers of ε . Taking small enough ε enables its approximation by a finite number of terms. At the same time, it should be borne in mind that the Magnus series as an expansion of logarithm may converge relatively slowly. Explicit estimates expressed in terms of ω, k_x and $\langle \mathbf{N} \rangle$ which ensure a desired accuracy of truncating the Magnus series up to a given order are formulated in Appendix A.

The structure of polynomial dependence of the Magnus series terms $\mathbf{K}^{(m)}$ on k_x and ω^2 is

$$\begin{aligned} \mathbf{K}^{(1)} &= i \begin{pmatrix} k_x^2 \mathbf{a}_1^{(1)} + \omega^2 \mathbf{a}_2^{(1)} & k_x \mathbf{a}_3^{(1)} \\ k_x(k_x^2 \mathbf{a}_4^{(1)} + \omega^2 \mathbf{a}_5^{(1)}) & -k_x^2 \mathbf{a}_1^{(1)\text{T}} - \omega^2 \mathbf{a}_2^{(1)} \end{pmatrix}, \\ \mathbf{K}^{(2)} &= \begin{pmatrix} k_x(k_x^2 \mathbf{a}_1^{(2)} + \omega^2 \mathbf{a}_2^{(2)}) & k_x^2 \mathbf{a}_3^{(2)} + \omega^2 \mathbf{a}_4^{(2)} \\ k_x^2(k_x^2 \mathbf{a}_5^{(2)} + \omega^2 \mathbf{a}_6^{(2)}) + \omega^4 \mathbf{a}_7^{(2)} & k_x(k_x^2 \mathbf{a}_1^{(2)\text{T}} + \omega^2 \mathbf{a}_2^{(2)\text{T}}) \end{pmatrix}, \\ \mathbf{K}^{(3)} &= i \begin{pmatrix} k_x^2(k_x^2 \mathbf{a}_1^{(3)} + \omega^2 \mathbf{a}_2^{(3)}) + \omega^4 \mathbf{a}_3^{(3)} & k_x(k_x^2 \mathbf{a}_4^{(3)} + \omega^2 \mathbf{a}_5^{(3)}) \\ k_x(k_x^4 \mathbf{a}_6^{(3)} + \omega^2 k_x^2 \mathbf{a}_7^{(3)} + \omega^4 \mathbf{a}_8^{(3)}) & -k_x^2(k_x^2 \mathbf{a}_1^{(3)\text{T}} + \omega^2 \mathbf{a}_2^{(3)\text{T}}) - \omega^4 \mathbf{a}_3^{(3)\text{T}} \end{pmatrix} \text{ etc.}, \end{aligned} \quad (14)$$

where the real matrices $\mathbf{a}^{(m)}$ in $\mathbf{K}^{(m)}$ are $(m+1)$ -tuple integrals of appropriate commutators; for instance, $\mathbf{a}_i^{(1)}$ in $\mathbf{K}^{(1)}$ are

$$\begin{aligned} \{\mathbf{a}_1^{(1)}, \mathbf{a}_2^{(1)}, \mathbf{a}_3^{(1)}, \mathbf{a}_4^{(1)}, \mathbf{a}_5^{(1)}\} &= \frac{1}{2}T \int_0^1 d\tilde{\zeta} \int_0^{\tilde{\zeta}} d\tilde{\zeta}_1 \left\{ [\mathbf{N}_1, \mathbf{N}_1] + [\mathbf{N}_2, \mathbf{N}_3], [\rho \mathbf{I}, \mathbf{N}_2], \right. \\ &\quad \left. [\mathbf{N}_1, \mathbf{N}_2] + [\mathbf{N}_2, \mathbf{N}_1^{\text{T}}], [\mathbf{N}_3, \mathbf{N}_1] + [\mathbf{N}_1^{\text{T}}, \mathbf{N}_3], [\mathbf{N}_1 - \mathbf{N}_1^{\text{T}}, \rho \mathbf{I}] \right\}. \end{aligned} \quad (15)$$

The series terms $\mathbf{K}^{(m)}$ of odd and even order m are imaginary and real, respectively, and each term $\mathbf{K}^{(m)}$ on its own satisfies (11); therefore

$$\mathbf{K}^{(m)} = -\mathbf{K}^{(m)*} = -\mathbf{TK}^{(m)\text{T}}\mathbf{T} \text{ for odd } m, \quad \mathbf{K}^{(m)} = \mathbf{K}^{(m)*} = \mathbf{TK}^{(m)\text{T}}\mathbf{T} \text{ for even } m, \quad (16)$$

as taken into account in (14). According to (12),

$$\mathbf{K}^{(m)} = \mathbf{0} \text{ for odd } m, \text{ if } \mathbf{Q}(\tilde{y}) \text{ is symmetric.} \quad (17)$$

Note the pure dynamic imaginary terms proportional to $\pm i\omega^{m+1}$, which appear in the diagonal blocks of the series terms $\mathbf{K}^{(m)}$ of odd order m unless these are zero for a symmetric $\mathbf{Q}(\tilde{y})$ by (17).

2.3 Dynamic homogenization

According to the Floquet theorem (9), the wave field variation over a large distance y is characterized mainly by the function $\exp(i\mathbf{K}y)$ (which is an exact wave field at $y = nT$). Formally $\exp(i\mathbf{K}y)$

with $i\mathbf{K}T = \ln \mathbf{M}(T, 0)$ is a solution to Eq. (2) with the actual matrix of coefficients $\mathbf{Q}(y)$ replaced by the constant matrix $i\mathbf{K}$. This motivates the concept of an effective homogeneous medium, whose material model admits the wave equation in the form (2) with a constant system matrix $\mathbf{Q}_{\text{eff}} \equiv i\mathbf{K}$. Confining the Magnus series (13) to the zero-order term defines the statically averaged $\mathbf{Q}_{\text{eff}}^{(0)} = \langle \mathbf{Q} \rangle$ which fits (3) with $\mathbf{N}_{\text{eff}} = \langle \mathbf{N} \rangle$ and hence yields the non-dispersive effective density and stiffness in the well-known form $\rho^{(0)} = \langle \rho \rangle$ and

$$(nn)^{(0)} = -\langle \mathbf{N}_2 \rangle^{-1}, \quad (nm)^{(0)} = \langle \mathbf{N}_2 \rangle^{-1} \langle \mathbf{N}_1 \rangle, \quad (mm)^{(0)} = \langle \mathbf{N}_3 \rangle - \langle \mathbf{N}_1^T \rangle \langle \mathbf{N}_2 \rangle^{-1} \langle \mathbf{N}_1 \rangle, \quad (18)$$

see [5]. It is evident that the statically averaged $\mathbf{Q}_{\text{eff}}^{(0)} = \langle \mathbf{Q} \rangle$ completely ignores dynamic effects and is inadequate to describe waves at finite frequency over long propagation distance. Dynamic properties are realized by taking $\mathbf{Q}_{\text{eff}} = i\mathbf{K}$ beyond the zero-order term $\langle \mathbf{Q} \rangle$, see next Section. Note that, in contrast to $\langle \mathbf{Q} \rangle$, a dispersive $\mathbf{Q}_{\text{eff}} = i\mathbf{K}$ generally depends on where the reference point $y = 0$ of the period interval $[0, T]$ is chosen.

3 A dispersive effective medium with $\mathbf{Q}_{\text{eff}} = i\mathbf{K}$

3.1 The constitutive equations

Our purpose is to take into account the full nature of the wave number matrix in $\mathbf{Q}_{\text{eff}} = i\mathbf{K}$. With this in mind, compare the structure of the dispersive effective matrix as given by the Magnus expansion $\mathbf{Q}_{\text{eff}} = \langle \mathbf{Q} \rangle + i \sum_{m=1} \mathbf{K}^{(m)}$ with that of $\mathbf{Q}(y)$ given by (3). They differ in two ways. First, $\mathbf{Q}_{\text{eff}} (\neq \langle \mathbf{Q} \rangle)$ is no longer imaginary, and hence the identity $\mathbf{Q}_{\text{eff}} = -\mathbf{T}\mathbf{Q}_{\text{eff}}^+\mathbf{T}$ which leads to (11) (and ensures energy conservation) is no longer compatible with a Hamiltonian structure for \mathbf{Q}_{eff} . This is a well-known feature of dispersive models, see e.g. [17]. The second, more significant, dissimilarity is that, by contrast to (3), \mathbf{Q}_{eff} has pure dynamic terms on the diagonal, already at the first-order $i\mathbf{K}^{(1)}$, see (14). This means that assuming dispersive density and elastic constants does not allow the constitutive relations of the dispersive effective medium to be written in the standard form of equations (1). Recalling that the upper rows of the sextic system (2) imply the traction-strain law, it is seen that the latter must be complemented by a purely dynamic term which implies different constitutive relations than those of the inhomogeneous medium itself.

On this basis, following [13, 14], the equations of equilibrium and the constitutive relations (1) are replaced by the more general form proposed by Willis

$$\sigma_{ij,i} = \dot{p}_j, \quad \sigma_{ij} = c_{ijkl}^{(\text{eff})} e_{kl} + S_{ijr} \dot{u}_r, \quad p_q = S_{klq} e_{kl} + \rho_{qr}^{(\text{eff})} \dot{u}_r. \quad (19)$$

The vector \mathbf{p} generalizes the normal notion of momentum density, and the elements of the Willis coupling tensor satisfy $S_{ijk} = S_{jik}$ by assumption, ensuring the symmetry of the stress tensor. A principal objective is to show that setting $\mathbf{Q}_{\text{eff}} = i\mathbf{K}$ leads inevitably to dispersive effective matrix density $\rho^{(\text{eff})}$ and stiffness $c_{ijkl}^{(\text{eff})}$ and, on top of that, to the Willis form of the effective constitutive relations with stress-impulse coupling.

3.2 The effective Willis medium

Denote by \mathbf{S}_n and \mathbf{S}_m the matrices with components

$$(\mathbf{S}_n)_{jk} = n_i S_{ijk}, \quad (\mathbf{S}_m)_{jk} = m_i S_{ijk}. \quad (20)$$

The same derivation that led from (1) to the sextic system (2) with the coefficients (3) now leads from (19) to (2) with the system matrix

$$\mathbf{Q}_{\text{eff}} = i \begin{pmatrix} k_x \mathbf{N}_1^{(\text{eff})} - \omega \mathbf{N}_2^{(\text{eff})} \mathbf{S}_{\mathbf{n}} & \mathbf{N}_2^{(\text{eff})} \\ k_x^2 \mathbf{N}_3^{(\text{eff})} - \omega^2 (\boldsymbol{\rho}^{(\text{eff})} - \mathbf{S}_{\mathbf{n}}^+ \mathbf{N}_2^{(\text{eff})} \mathbf{S}_{\mathbf{n}}) - \omega k_x \mathbf{L} & k_x \mathbf{N}_1^{(\text{eff})+} - \omega \mathbf{S}_{\mathbf{n}}^+ \mathbf{N}_2^{(\text{eff})} \end{pmatrix}, \quad (21)$$

with $\mathbf{L} = \mathbf{S}_{\mathbf{n}}^+ \mathbf{N}_1^{(\text{eff})} + \mathbf{N}_1^{(\text{eff})+} \mathbf{S}_{\mathbf{n}} + \mathbf{S}_{\mathbf{m}} + \mathbf{S}_{\mathbf{m}}^+ = \mathbf{L}^+$. The identity $\mathbf{Q}_{\text{eff}} = -\mathbf{T} \mathbf{Q}_{\text{eff}}^+ \mathbf{T}$ is assumed in order to ensure that the effective medium is, like the inhomogeneous periodic medium, non-dissipative (energy conserving). This implies hermiticity constraints on the complex-valued material parameters: $\mathbf{c}^{(\text{eff})} = \mathbf{c}^{(\text{eff})+}$, $\boldsymbol{\rho}^{(\text{eff})} = \boldsymbol{\rho}^{(\text{eff})+}$, $\mathbf{S}_{\mathbf{n}} = -\mathbf{S}_{\mathbf{n}}^*$, $\mathbf{S}_{\mathbf{m}} = -\mathbf{S}_{\mathbf{m}}^*$, where $\mathbf{c}^{(\text{eff})}$ is the 6×6 stiffness matrix in Voigt's notation. The coupling tensor S_{ijk} is therefore purely imaginary. Note that the blocks $\mathbf{N}_J^{(\text{eff})}$ of the effective Stroh matrix $\mathbf{N}_{\text{eff}} = \mathbf{T} \mathbf{N}_{\text{eff}}^+ \mathbf{T} (\neq \mathbf{T} \mathbf{N}_{\text{eff}}^T \mathbf{T})$ consist of submatrices $(nn)^{(\text{eff})}$, $(nm)^{(\text{eff})}$, $(mm)^{(\text{eff})}$ built from $\mathbf{c}^{(\text{eff})}$ according to the definition (4) but with $(mn)^{(\text{eff})} = (nm)^{(\text{eff})+}$ so that $\mathbf{N}_4^{(\text{eff})} = \mathbf{N}_1^{(\text{eff})+}$.

Equating the matrix \mathbf{Q}_{eff} introduced in (21) to the matrix $i\mathbf{K}(\omega^2, k_x)$ with the block structure (11) yields the blockwise equalities

$$\begin{aligned} k_x \mathbf{N}_1^{(\text{eff})} - \omega \mathbf{N}_2^{(\text{eff})} \mathbf{S}_{\mathbf{n}} &= \mathbf{K}_1, & \mathbf{N}_2^{(\text{eff})} &= \mathbf{K}_2, \\ k_x^2 \mathbf{N}_3^{(\text{eff})} - \omega^2 (\boldsymbol{\rho}^{(\text{eff})} - \mathbf{S}_{\mathbf{n}}^+ \mathbf{N}_2^{(\text{eff})} \mathbf{S}_{\mathbf{n}}) - \omega k_x \mathbf{L} &= \mathbf{K}_3. \end{aligned} \quad (22)$$

Identification of the effective parameters based on these identities is ambiguous given that they may depend upon both ω and k_x . A unique and arguably the simplest solution is obtained by first assuming a purely dynamic $S_{ijk} = S_{ijk}(\omega)$. Then (22₁) and (22₂) yield

$$\omega \mathbf{S}_{\mathbf{n}} = -\mathbf{K}_2^{-1}(0) \mathbf{K}_1(0), \quad (nn)^{(\text{eff})} = -\mathbf{K}_2^{-1}, \quad k_x (nm)^{(\text{eff})} = \mathbf{K}_2^{-1} \mathbf{K}_1 - \mathbf{K}_2^{-1}(0) \mathbf{K}_1(0), \quad (23)$$

where the blocks $\mathbf{K}_J(\omega^2, k_x)$ of \mathbf{K} are taken at $k_x = 0$ as indicated by the notation $\mathbf{K}_J(0) \equiv \mathbf{K}_J(\omega^2, 0)$ used here and subsequently. Note that the validity of (23) requires the block \mathbf{K}_2 to be invertible which is assumed in the following. For \mathbf{K} defined by the Magnus series (13), the conditions that ensure existence of \mathbf{K}_2^{-1} in a certain low-frequency long-wave range and the estimates that enable truncation of its expansion are established in Appendix A. In view of (23), the remaining identity (22₃) becomes

$$k_x^2 (mm)^{(\text{eff})} - \omega^2 \boldsymbol{\rho}^{(\text{eff})} - \omega k_x (\mathbf{S}_{\mathbf{m}} + \mathbf{S}_{\mathbf{m}}^+) = \mathbf{K}_3 - \mathbf{K}_1^+ \mathbf{K}_2^{-1} \mathbf{K}_1. \quad (24)$$

Pursuing the logical extension of the assumed dependence of the inertial coupling tensor \mathbf{S} on frequency alone, we assume that the inertia tensor $\boldsymbol{\rho}^{(\text{eff})}$ is also purely dynamic. This leads to a unique solution of (24) since $\boldsymbol{\rho}^{(\text{eff})} = \boldsymbol{\rho}^{(\text{eff})}(\omega)$ is found by setting $k_x = 0$,

$$-\omega (\mathbf{S}_{\mathbf{m}} + \mathbf{S}_{\mathbf{m}}^+) = \lim_{k_x \rightarrow 0} k_x^{-1} \{ \mathbf{K}_3 - \mathbf{K}_1^+ \mathbf{K}_2^{-1} \mathbf{K}_1 - (\mathbf{K}_3(0) - \mathbf{K}_1^+(0) \mathbf{K}_2^{-1}(0) \mathbf{K}_1(0)) \}. \quad (25)$$

The limit may be achieved in terms of derivatives of matrices \mathbf{K}_J at $k_x = 0$, whose existence is guaranteed for instance within the range of convergence of the Magnus expansion. Accordingly, the solutions of (24) are

$$\begin{aligned} \omega^2 \boldsymbol{\rho}^{(\text{eff})} &= \mathbf{K}_1^+(0) \mathbf{K}_2^{-1}(0) \mathbf{K}_1(0) - \mathbf{K}_3(0), \\ \omega (\mathbf{S}_{\mathbf{m}} + \mathbf{S}_{\mathbf{m}}^+) &= -\mathbf{K}_3'(0) - \omega \mathbf{S}_{\mathbf{n}}^+ \mathbf{K}_1'(0) - \omega \mathbf{K}_1^{+'}(0) \mathbf{S}_{\mathbf{n}} - \omega^2 \mathbf{S}_{\mathbf{n}}^+ \mathbf{K}_2'(0) \mathbf{S}_{\mathbf{n}}, \\ k_x^2 (mm)^{(\text{eff})} &= \mathbf{K}_3 - \mathbf{K}_1^+ \mathbf{K}_2^{-1} \mathbf{K}_1 + \omega^2 \boldsymbol{\rho}^{(\text{eff})} + \omega k_x (\mathbf{S}_{\mathbf{m}} + \mathbf{S}_{\mathbf{m}}^+). \end{aligned} \quad (26)$$

where $\mathbf{K}'_J(0) = \partial \mathbf{K}_J(\omega^2, k_x) / \partial k_x \big|_{k_x=0}$.

In summary, Eqs. (23) and (26) provide unique material properties for the Willis model with

$$\mathbf{c}^{(\text{eff})}(\omega, k_x) = \mathbf{c}^{(\text{eff})+}, \quad \boldsymbol{\rho}^{(\text{eff})}(\omega) = \boldsymbol{\rho}^{(\text{eff})+}, \quad \mathbf{S}(\omega) = -\mathbf{S}^*, \quad (27)$$

and $S_{ijk} = S_{jik}$. The lack of dependence of the inertial parameters on k_x means that non-local effects are confined to the elastic moduli $\mathbf{c}^{(\text{eff})}$. The result reduces to non-dispersive statically averaged moduli of (18) with $\boldsymbol{\rho}^{(\text{eff})} = \langle \rho \rangle \mathbf{I}$ and $\mathbf{S} = \mathbf{0}$ when $i\mathbf{K}$ is restricted to the zero-order term $\langle \mathbf{Q} \rangle$ of (13).

Regarding computation of the Willis parameters from Eqs. (23) and (26), it is assumed that the wavenumber matrix $\mathbf{K}(\omega^2, k_x)$ defined as $i\mathbf{K}T = \ln \mathbf{M}(T, 0)$ is known either in the form of long-wave low-frequency series, or from the direct definition of matrix logarithm in some neighbourhood of a given point ω, k_x (see the example in §4). In particular, one may first evaluate the matricant $\mathbf{M}(T, 0)$ numerically and \mathbf{K} then follows from the matrix logarithm. The matrix $\mathbf{K}'(0)$, required for the solution of Eq. (26)₂, involves evaluating the derivative of $\ln \mathbf{M}(T, 0)$ in k_x . It may be expressed using either series or integral representation of $\ln \mathbf{M}$ as

$$\ln \mathbf{M} = - \sum_{n=1}^{\infty} \frac{1}{n} (\mathbf{I} - \mathbf{M})^n = (\mathbf{M} - \mathbf{I}) \int_0^1 [x(\mathbf{M} - \mathbf{I}) + \mathbf{I}]^{-1} dx, \quad (28)$$

which leads to

$$i\mathbf{K}'(0)T = \sum_{n=1}^{\infty} \frac{1}{n} (-1)^{n-1} \sum_{j=0}^{n-1} \mathbf{A}^j \mathbf{M}'(0) \mathbf{A}^{n-1-j} = \int_0^1 [x\mathbf{A} + \mathbf{I}]^{-1} \mathbf{M}'(0) [x\mathbf{A} + \mathbf{I}]^{-1} dx, \quad (29)$$

with $\mathbf{A} = \mathbf{M}(T, 0) - \mathbf{I}$ at $k_x = 0$, and the derivative of the matricant itself is [2]

$$\mathbf{M}'(0) \equiv \left. \frac{\partial \mathbf{M}(T, 0)}{\partial k_x} \right|_{k_x=0} = i \int_0^T \mathbf{M}(T, \tilde{\zeta}) \begin{pmatrix} \mathbf{N}_1 & 0 \\ 0 & \mathbf{N}_1^T \end{pmatrix} \mathbf{M}(\tilde{\zeta}, 0) d\tilde{\zeta}. \quad (30)$$

The sufficient conditions for the range of validity of the above series and integral definitions of $\mathbf{K}'(0)$ are specified in Appendix A.

3.3 Discussion

3.3.1 The Willis equation and its inertial quantities

Consider the above results (23) and (26) in more detail. Anisotropic density and the coupling coefficients that relate particle momentum and stress are unknown in "standard" models of solids. Here they appear as inevitable ingredients of a model that replaces periodic spatial inhomogeneity with a spatially homogeneous but dispersive and non-local theory. The departure from normal elasticity is evident from the equations of motion for the displacement that follows from (19),

$$c_{ijkl}^{(\text{eff})} u_{l,ik} + (S_{ijl} - S_{ilj}) \dot{u}_{l,i} - \rho_{jl}^{(\text{eff})} \ddot{u}_l = 0. \quad (31)$$

This in turn leads to an energy conservation equation of the form $\dot{U} + \text{div } \mathbf{f} = 0$ where the real-valued energy density and flux vector are

$$U = \frac{1}{2} c_{ijkl}^{(\text{eff})} u_{l,k} u_{j,i}^* + \frac{1}{2} \rho_{jl}^{(\text{eff})} \dot{u}_l \dot{u}_j^*, \quad f_i = -\frac{1}{2} (S_{ijl} - S_{ilj}) \dot{u}_l \dot{u}_j^* - \text{Re}(c_{ijkl}^{(\text{eff})} u_{l,k} \dot{u}_j^*). \quad (32)$$

In order to gain some insight into these new dynamic terms, consider a layered transversely isotropic medium, with the principal axis along \mathbf{n} identified as the 2-direction. The effective density is of the form $\boldsymbol{\rho}^{(\text{eff})} = \text{diag}(\rho_{11}^{(\text{eff})}, \rho_{22}^{(\text{eff})}, \rho_{11}^{(\text{eff})})$ and the only non-zero elements of the coupling tensor (up to symmetries $S_{ijk} = S_{jik}$) are $S_{112} = S_{332}$, $S_{211} = S_{233}$ and S_{222} . Only one combination of the three independent coupling elements has impact on the equations of motion,

$$\begin{aligned} c_{ijkl}^{(\text{eff})} u_{l,ik} + (S_{112} - S_{211}) \dot{u}_{2,j} - \rho_{11}^{(\text{eff})} \ddot{u}_j &= 0, \quad j = 1, 3, \\ c_{2kl}^{(\text{eff})} u_{l,ik} + (S_{211} - S_{112})(\dot{u}_{1,1} + \dot{u}_{3,3}) - \rho_{22}^{(\text{eff})} \ddot{u}_2 &= 0, \end{aligned} \tag{33}$$

and it has no influence on pure SH wave motion (polarized in the plane orthogonal to \mathbf{n}). Long-wave expansions of $\rho_{jj}^{(\text{eff})}$ and S_{ijk} are presented in (34). Further detailed discussion for SH waves is provided in §4.

More generally, the absence of generating functions for $\mathbf{S}_m - \mathbf{S}_m^+$ means that some elements of the Willis coupling tensor S_{ijk} should be set to zero in order to complete its definition. The relevant elements are necessary to determine stress and momentum but do not enter into the equation of motion (31) and the sextic system (2) with (21) because the purely imaginary property of the coupling tensor means that $m_i(S_{ijl} - S_{ilj})$ are the elements of $\mathbf{S}_m + \mathbf{S}_m^+$. Consider the two dimensional situation with indices taking only two values so that, on account of the symmetry $S_{ijk} = S_{jik}$, there are at most six independent elements. Four of these may be found from (23)₁, and one more follows from (26)₂ using the symmetry property. The single element $\mathbf{m} \cdot \mathbf{S}_m \mathbf{m}$ is undefined and may be set equal to zero. In the three dimensional situation all but four combinations of the 18 independent elements of S_{ijk} are obtainable. Taking an orthonormal triad $\{\mathbf{m}_1, \mathbf{n}, \mathbf{m}_2\}$, the following elements of the coupling tensor are not defined by the effective medium equations and are therefore set to zero: $\mathbf{m}_\alpha \cdot \mathbf{S}_{m_\alpha} \mathbf{m}_\beta + \mathbf{m}_\beta \cdot \mathbf{S}_{m_\alpha} \mathbf{m}_\alpha$, $\alpha, \beta \in \{1, 2\}$. To be explicit, let \mathbf{n} lie in the 2-direction, then the \mathbf{S}_n equation (23)₁ defines the nine elements S_{2jk} ; these combined with the $\mathbf{S}_m + \mathbf{S}_m^+$ equations (26)₂ yield S_{112} , S_{132} , S_{32} , and the $\mathbf{S}_m + \mathbf{S}_m^+$ equations with the above prescriptions give $S_{113} = -S_{131}$, $S_{313} = -S_{331}$, $S_{111} = 0$, $S_{333} = 0$.

3.3.2 Expansion of the Willis parameters

Explicit insight into the structure of the Willis parameters can be gained from their expansion obtained via the Magnus series for the wave number matrix \mathbf{K} . In view of (14) and (16), $\mathbf{K}_1(0)$ is imaginary and expands as $\mathbf{K}_1(0) = \sum_m \mathbf{K}_1^{(m)}(0)$ with odd m and $\mathbf{K}_1^{(m)}(0) \sim i\omega^{m+1}$, while $\mathbf{K}_2(0)$ is real and expands as $\mathbf{K}_2(0) = \langle \mathbf{N}_2 \rangle + \sum_m \mathbf{K}_2^{(m)}(0)$ with even m and $\mathbf{K}_2^{(m)}(0) \sim \omega^m$. This confirms that \mathbf{S}_n is imaginary and vanishes at $\omega = 0$. It is easy to check that the right-hand sides of (23)₃ and (24) are zero at $k_x = 0$ and at ω , $k_x = 0$, respectively. Based on the forms of $\mathbf{K}_J(\omega^2, k_x)$ as generated by the Magnus expansion, and evident from (14) for the leading order contributions, it may be demonstrated that (26)₂ is consistent with imaginary \mathbf{S}_m that is zero at $\omega = 0$. It is noteworthy that keeping the density $\boldsymbol{\rho}^{(\text{eff})}$ as $\langle \rho \rangle$ or as any other scalar is generally not possible since this would contradict the pure dynamic term on the right-hand side of (24). Finally, it is emphasized that, by virtue of (17), the stress-impulse tensor defined as a pure dynamic quantity $S_{ijk} = S_{ijk}(\omega)$ vanishes in the case of a unit cell with any symmetric heterogeneity profile $\mathbf{Q}(\tilde{y})$ (regarding the "inaccessible" part $\mathbf{S}_m - \mathbf{S}_m^+$, see §3.3.1).

Equations (23) and (26) with polynomials $\mathbf{K}_J(\omega^2, k_x)$ given by the Magnus series (13) imply that the elastic moduli $c_{ijkl}^{(\text{eff})}$ are rational functions of ω^2, k_x while the density and coupling terms

$\boldsymbol{\rho}^{(\text{eff})}$, ωS_{ijk} are functions of ω^2 , defined by the series

$$\{\mathbf{c}^{(\text{eff})}(\omega^2, k_x), \boldsymbol{\rho}^{(\text{eff})}(\omega^2), \mathbf{S}(\omega)\} = \{\mathbf{c}^{(0)}, \langle \rho \rangle \mathbf{I}, 0\} + \sum_{m=1,2,\dots} \{\mathbf{c}^{(m)}, \boldsymbol{\rho}^{(2m)}, \mathbf{S}^{(2m-1)}\}, \quad (34)$$

with real $\boldsymbol{\rho}^{(m)}$ and imaginary $S_{ijk}^{(m)}$ proportional to ω^m , $c_{ijkl}^{(m)}$ real or imaginary depending as m is odd or even, respectively. These series are similar to (13) in that they are majorised by the power series in long-wave parameter ε . The Magnus series with M terms enables finding M terms of the series (34). It is apparent from (23₁), (26₁) and (3) that \mathbf{S}_n and $\boldsymbol{\rho}^{(\text{eff})}$ depend only upon \mathbf{N}_2 and ρ , thus

$$\begin{aligned} \mathbf{S}_n(\omega) &= -i\omega \langle \mathbf{N}_2 \rangle^{-1} \{ \mathbf{a}_2^{(1)} + \omega^2 (\mathbf{a}_3^{(3)} - \mathbf{a}_4^{(2)} \langle \mathbf{N}_2 \rangle^{-1} \mathbf{a}_2^{(1)}) + \dots \}, \\ \boldsymbol{\rho}^{(\text{eff})}(\omega) &= \langle \rho \rangle \mathbf{I} - \omega^2 (\mathbf{a}_7^{(2)} - \mathbf{a}_2^{(1)} \langle \mathbf{N}_2 \rangle^{-1} \mathbf{a}_2^{(1)}) + \dots, \end{aligned} \quad (35)$$

with

$$\begin{aligned} \mathbf{a}_2^{(1)} &= \frac{T}{2} \int_0^1 \int_0^{\tilde{\zeta}} (\rho \mathbf{N}_2 - \mathbf{N}_2 \rho) \quad (= \mathbf{a}_2^{(1)\text{T}}), \\ \{\mathbf{a}_4^{(2)}, \mathbf{a}_7^{(2)} (= \mathbf{a}_7^{(2)\text{T}})\} &= \frac{T^2}{6} \int_0^1 \int_0^{\tilde{\zeta}} \int_0^{\tilde{\zeta}_1} \{ 2\mathbf{N}_2 \rho \mathbf{N}_2 - \mathbf{N}_2 \mathbf{N}_2 \rho - \rho \mathbf{N}_2 \mathbf{N}_2, \rho \rho \mathbf{N}_2 + \mathbf{N}_2 \rho \rho - 2\rho \mathbf{N}_2 \rho \}, \\ \mathbf{a}_3^{(3)} &= \frac{T^3}{6} \int_0^1 \int_0^{\tilde{\zeta}} \int_0^{\tilde{\zeta}_1} \int_0^{\tilde{\zeta}_2} (2\rho \mathbf{N}_2 \rho \mathbf{N}_2 - 2\mathbf{N}_2 \rho \mathbf{N}_2 \rho + \mathbf{N}_2 \mathbf{N}_2 \rho \rho - \rho \rho \mathbf{N}_2 \mathbf{N}_2), \end{aligned} \quad (36)$$

in which $d\tilde{\zeta}$, $d\tilde{\zeta}_1, \dots$ are suppressed (as kept tacit hereafter) and dependence of co-factors on the successive integration variables $\tilde{\zeta}$, $\tilde{\zeta}_1, \dots$ is understood. The remaining part of the coupling tensor is only obtainable through the combination $\mathbf{S}_m + \mathbf{S}_m^+$, and it depends upon \mathbf{N}_1 , \mathbf{N}_2 and ρ , with

$$\begin{aligned} \mathbf{S}_m + \mathbf{S}_m^+ &= i\omega (\langle \mathbf{N}_1 \rangle^{\text{T}} \langle \mathbf{N}_2 \rangle^{-1} \mathbf{a}_2^{(1)} - \mathbf{a}_2^{(1)} \langle \mathbf{N}_2 \rangle^{-1} \langle \mathbf{N}_1 \rangle^{\text{T}} - \mathbf{a}_5^{(1)}) + O(\omega^3), \quad \text{where} \\ \mathbf{a}_5^{(1)} &= \frac{1}{2} T \int_0^1 \int_0^{\tilde{\zeta}} ((\mathbf{N}_1 - \mathbf{N}_1^{\text{T}}) \rho - \rho (\mathbf{N}_1 - \mathbf{N}_1^{\text{T}})) \quad (= -\mathbf{a}_5^{(1)\text{T}}). \end{aligned} \quad (37)$$

For example, the expansions of the inertial quantities for the transversely isotropic layered medium discussed in §3.3.2 are $\boldsymbol{\rho}^{(\text{eff})} = \langle \rho \rangle \mathbf{I} + \boldsymbol{\rho}^{(2)} + \dots$

$$\begin{aligned} \rho_{22}^{(2)} &= (\omega T)^2 \left\{ \frac{1}{6} \int_0^1 \int_0^{\tilde{\zeta}} \int_0^{\tilde{\zeta}_1} (\rho \rho c_{22}^{-1} + c_{22}^{-1} \rho \rho - 2\rho c_{22}^{-1} \rho) - \langle c_{22}^{-1} \rangle^{-1} \left(\frac{1}{2} \int_0^1 \int_0^{\tilde{\zeta}} (c_{22}^{-1} \rho - \rho c_{22}^{-1}) \right)^2 \right\}, \\ S_{222}^{(1)} &= \frac{i}{2} \omega T \langle c_{22}^{-1} \rangle^{-1} \int_0^1 \int_0^{\tilde{\zeta}} (c_{22}^{-1} \rho - \rho c_{22}^{-1}), \\ S_{112}^{(1)} &= \frac{i}{2} \omega T \left\{ \left\langle \frac{c_{12}}{c_{22}} \right\rangle^{-1} \langle c_{22}^{-1} \rangle^{-1} \int_0^1 \int_0^{\tilde{\zeta}} (c_{22}^{-1} \rho - \rho c_{22}^{-1}) + \int_0^1 \int_0^{\tilde{\zeta}} \left(\left(1 - \frac{c_{12}}{c_{22}} \right) \rho - \rho \left(1 - \frac{c_{12}}{c_{22}} \right) \right) \right\}, \end{aligned} \quad (38)$$

and $\rho_{11}^{(2)}$, $S_{211}^{(1)} = S_{233}^{(1)}$ have respectively the same form as $\rho_{22}^{(2)}$, $S_{222}^{(1)}$ with c_{22} replaced by c_{66} in (38)_{1,2}.

3.3.3 Effective medium defined from the Floquet dispersion

Modelling a dispersive effective medium may be based on a more relaxed approach that abandons fitting the matrix $i\mathbf{K}$ to the coefficients of sextic system of wave equations and deals instead with the asymptotic secular equation for the eigenvalues iK_α or $e^{iK_\alpha T}$ of $i\mathbf{K}$ or $\mathbf{M}(T, 0)$, which is a

dispersion equation for the onset of fundamental Floquet branches $K_\alpha(\omega, k_x)$ or $\omega_\alpha(k_x, K)$ analyzed in [5, 6, 7]. This gives the same secular equation as that for the $i\mathbf{K}$ matrices, and hence preserves the long-wave Floquet dispersion but not the displacement-traction vector \mathbf{w}_α at the period edges (see (10)). By not fitting all of the physical properties, this type of approach to homogenization modelling introduces extra degrees of freedom. In particular, a "modified" effective medium may be defined that is asymptotically similar to $i\mathbf{K}$ but the matrix $\tilde{\mathbf{Q}}_{\text{eff}}$ has no pure dynamic terms in the diagonal blocks, and hence matches the Stroh-like form (3), (4) (though now with $(27)_1$), i.e. satisfies the standard form of the governing equations (1) with dispersive effective coefficients.

For instance, in the 1D case $k_x = 0$, the matrix

$$\mathbf{Q}_{\text{eff}} = \langle \mathbf{Q} \rangle + i\mathbf{K}^{(1)} + i\mathbf{K}^{(2)} = i \begin{pmatrix} i\omega^2 \mathbf{a}_2^{(1)} & \langle \mathbf{N}_2 \rangle + \omega^2 \mathbf{a}_4^{(2)} \\ -\langle \rho \rangle \omega^2 \mathbf{I} + \omega^4 \mathbf{a}_7^{(2)} & -i\omega^2 \mathbf{a}_2^{(1)} \end{pmatrix} \quad (39)$$

has asymptotically (to the order of this matrix itself) the same secular equation as the matrix

$$\tilde{\mathbf{Q}}_{\text{eff}} = i \begin{pmatrix} \mathbf{0} & \langle \mathbf{N}_2 \rangle + \omega^2 \mathbf{a}_4^{(2)} \\ -\langle \rho \rangle \omega^2 \mathbf{I} + \omega^4 (\mathbf{a}_7^{(2)} - \mathbf{a}_2^{(1)2} \langle \mathbf{N}_2 \rangle^{-1}) & \mathbf{0} \end{pmatrix}. \quad (40)$$

The latter "skips" (by construction) the Willis coupling tensor and leads to the same definition of the matrix of second-order elastic coefficients $(nn)^{(2)}$ as in (23), while the second-order density matrix $\tilde{\boldsymbol{\rho}}^{(2)} = \omega^2 (\mathbf{a}_2^{(1)2} \langle \mathbf{N}_2 \rangle^{-1} - \mathbf{a}_7^{(2)})$ following from (40) is generally different from $\boldsymbol{\rho}^{(2)}$ in (35) due to non-commutativity of $\langle \mathbf{N}_2 \rangle$ and $\mathbf{a}_2^{(1)}$. See also the SH example in Appendix B.

4 Effective medium coefficients for SH waves

4.1 The wave number matrix

Consider SH waves in an isotropic medium with periodic density $\rho(y)$ and shear modulus $\mu(y)$. The SH state vector $\boldsymbol{\eta}(y) = (A, iF)^T$, where A and F are the amplitudes of $u = u_3$ and σ_{23} (the indices correspond to $\mathbf{u} \parallel X_3$, $\mathbf{n} \parallel X_2$, $\mathbf{m} \parallel X_1$), satisfies Eq. (2) with the system matrix

$$\mathbf{Q}(y) = i \begin{pmatrix} 0 & -\mu^{-1} \\ \mu k_x^2 - \rho \omega^2 & 0 \end{pmatrix}. \quad (41)$$

The 2×2 case leads to some simplifications not available for higher algebraic dimensions. In particular, the two eigenvalues of the monodromy matrix $\mathbf{M}(T, 0)$, which are the inverse of one other (since $\det \mathbf{M} = 1$ due to the isotropy), are defined by the single quantity $\text{tr} \mathbf{M}(T, 0)$. The implications are explored in [15] and only the necessary equations are cited here - the reader is referred to [15] for details. The main result is that the wave number matrix, and hence the effective system matrix $\mathbf{Q}_{\text{eff}}(\omega) = i\mathbf{K}$ has semi-explicit form,

$$\mathbf{Q}_{\text{eff}} = i \begin{pmatrix} K_1 & K_2 \\ K_3 & -K_1 \end{pmatrix} = \frac{K}{\sin KT} [\mathbf{M}(T, 0) - \mathbf{I} \cos KT], \quad KT = \cos^{-1} \left(\frac{1}{2} \text{tr} \mathbf{M}(T, 0) \right), \quad (42)$$

where $\text{Re} \cos^{-1} \in [0, \pi]$, $\text{Im} \cos^{-1} \geq 0$, and $\pm K$ (no subscript) are the eigenvalues of \mathbf{K} .

4.2 Willis equations and effective coefficients

Following the general formalism of §3 the effective material is assumed to have constitutive equations described by the Willis model, which in this case has only a single momentum component p_3 and the usual stress components for SH waves in elasticity. Noting that $S_{53} = 0$, on account of the transversely isotropic axis \mathbf{n} , we have

$$\begin{pmatrix} \sigma_{13} \\ \sigma_{23} \\ p_3 \end{pmatrix} = \begin{pmatrix} c_{55}^{(\text{eff})} & c_{54}^{(\text{eff})} & 0 \\ c_{45}^{(\text{eff})} & c_{44}^{(\text{eff})} & S_{43} \\ 0 & S_{43} & \rho^{(\text{eff})} \end{pmatrix} \begin{pmatrix} u_{,1} \\ u_{,2} \\ \dot{u} \end{pmatrix}. \quad (43)$$

These constitutive relations imply, using (19₁), that the governing equation for the SH displacement is of the form

$$c_{44}^{(\text{eff})} u'' + (\omega^2 \rho^{(\text{eff})} - k_x^2 c_{55}^{(\text{eff})}) u = 0, \quad (44)$$

where $'$ means d/dy . The coupling term S_{43} is absent from the equation of motion, as expected from the Willis equations (19) for a scalar problem. At the same time, (43) leads to the state-vector system matrix in the form

$$\mathbf{Q}_{\text{eff}} = i \begin{pmatrix} -c_{44}^{(\text{eff})^{-1}} (k_x c_{45}^{(\text{eff})} - \omega S_{43}) & -c_{44}^{(\text{eff})^{-1}} \\ k_x^2 c_{55}^{(\text{eff})} - \omega^2 \rho^{(\text{eff})} + c_{44}^{(\text{eff})^{-1}} (k_x c_{45}^{(\text{eff})} - \omega S_{43})^2 & c_{44}^{(\text{eff})^{-1}} (k_x c_{45}^{(\text{eff})} - \omega S_{43}) \end{pmatrix}, \quad (45)$$

where $c_{45}^{(\text{eff})+} = c_{54}^{(\text{eff})} = -c_{45}^{(\text{eff})}$ has been used.

Setting \mathbf{Q}_{eff} of the Willis model equal to that of (42) gives the material parameters

$$\begin{aligned} c_{44}^{(\text{eff})} &= -K_2^{-1}, & \rho^{(\text{eff})} &= -\omega^{-2} (K_3(0) + K_2^{-1}(0) K_1^2(0)), & S_{43} &= -\omega^{-1} K_2^{-1}(0) K_1(0), \\ c_{55}^{(\text{eff})} &= k_x^{-2} (K_3 + K_2^{-1} K_1^2 + \omega^2 \rho^{(\text{eff})}), & c_{45}^{(\text{eff})} &= k_x^{-1} (K_2^{-1} K_1 - K_2^{-1}(0) K_1(0)), \end{aligned} \quad (46)$$

with $K_J(0) = K_J(\omega, 0)$. These may be expressed directly in terms of the elements of the monodromy matrix, using the form (42) along with $\det \mathbf{K} = -K^2$,

$$\begin{aligned} c_{44}^{(\text{eff})} &= \frac{\sin KT}{iKM_2}, & \rho^{(\text{eff})} &= \frac{K^2(0)}{\omega^2} c_{44}^{(\text{eff})}(0), & S_{43} &= \frac{M_4(0) - M_1(0)}{2\omega M_2(0)}, \\ c_{55}^{(\text{eff})} &= k_x^{-2} (\omega^2 \rho^{(\text{eff})} - K^2 c_{44}^{(\text{eff})}), & c_{45}^{(\text{eff})} &= k_x^{-1} (\omega S_{43} + \frac{M_1 - M_4}{2M_2}), \end{aligned} \quad (47)$$

where $M_J = M_J(T, 0)$ are functions of ω and k_x , and (0) means evaluated at $k_x = 0$. Note that the expressions for $\rho^{(\text{eff})}$ and $c_{55}^{(\text{eff})}$ also follow from the equation of motion (44) and its solution $u(y) = u(0)e^{iKy}$, using $k_x = 0$ for $\rho^{(\text{eff})}(\omega)$.

Explicit expressions for the low-frequency long-wave expansion of the material parameters may be found in the same manner as in §3.3.2 for the general case. The starting point is the Magnus expansion $\mathbf{Q}_{\text{eff}} = \langle \mathbf{Q} \rangle + i\mathbf{K}^{(1)} + i\mathbf{K}^{(2)}$ for the SH wave number matrix. Details of the analysis and a summary of the results are presented in Appendix B.

4.3 Examples and discussion

4.3.1 A bilayered unit cell

The general formulation is illustrated by the case of a two-component piecewise constant unit cell. Specifically, consider a periodic structure of homogeneous isotropic layers $j = 1, 2$, each

with constant density ρ_j , shear modulus μ_j and thickness d_j . The monodromy matrix $\mathbf{M}(T, 0) = e^{\mathbf{Q}_2 d_2} e^{\mathbf{Q}_1 d_1} \equiv \mathbf{M}(\omega, k_x)$ has the well-known form

$$\mathbf{M}(\omega, k_x) = \begin{pmatrix} \cos \psi_2 \cos \psi_1 - \frac{\gamma_1}{\gamma_2} \sin \psi_2 \sin \psi_1 & -\frac{i}{\gamma_1} \cos \psi_2 \sin \psi_1 - \frac{i}{\gamma_2} \sin \psi_2 \cos \psi_1 \\ -i\gamma_1 \cos \psi_2 \sin \psi_1 - i\gamma_2 \sin \psi_2 \cos \psi_1 & \cos \psi_2 \cos \psi_1 - \frac{\gamma_2}{\gamma_1} \sin \psi_2 \sin \psi_1 \end{pmatrix}, \quad (48)$$

where $\psi_j = d_j \sqrt{\mu_j^{-1} \rho_j \omega^2 - k_x^2}$ is the phase shift over a layer and $\gamma_j = \mu_j \psi_j / d_j$, see [15]. Figures 1

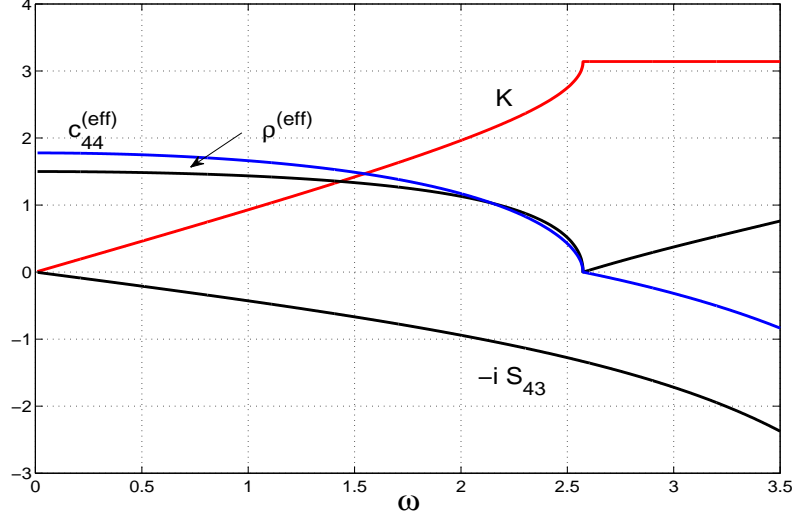


Figure 1: The effective material properties of the bilayered SH case for $k_x = 0$: elastic moduli, inertial parameters and the effective wave number are plotted in blue, black and red, respectively. The frequency range includes the first band edge which is at the frequency where $\text{Re } K = \pi$ first occurs. Only the real parts of the quantities indicated are plotted. For frequencies in the stop band the imaginary parts of $c_{44}^{(\text{eff})}$, $\rho^{(\text{eff})}$ and K are non-zero but not shown.

and 2 show the computed parameters for the case of layers of equal thickness, $d_1 = d_2 = 1/2$, with $\rho_1 = 1$, $c_1 = 1$; $\rho_2 = 2$, $c_2 = 2$, where c_j is the shear wave speed ($c^2 = \mu/\rho$). Figure 1 shows the effective parameters for propagation normal to the layers ($k_x = 0$). The vanishing of both $c_{44}^{(\text{eff})}$ and $\rho^{(\text{eff})}$ at the band edge at $\omega = \omega_1 \approx 2.6$ is expected on the basis of the fact that \mathbf{Q}_{eff} is singular at the band edge and scales as $(\omega - \omega_1)^{-1/2}$ near it [15]. Referring to the 12-element in Eq. (45), this implies first that $c_{44}^{(\text{eff})} \propto (\omega - \omega_1)^{1/2}$ and then, from the 21-element and the finite value of $\det \mathbf{Q}_{\text{eff}}$, that $\rho^{(\text{eff})} \propto (\omega - \omega_1)^{1/2}$. The square root decay of both $c_{44}^{(\text{eff})}$ and $\rho^{(\text{eff})}$ is apparent in Figure 1.

The wavenumber is finite, $k_x = 1$, in Figure 2. This has the effect of increasing the frequency of the band edge, and introducing a range of frequency from $\omega = 0$ up to the cut-on at $\omega \approx 1.7$ in which the effective wave is non-propagating. Note that $\rho^{(\text{eff})}$ and S_{43} are unchanged from Figure 1 while the elastic modulus $c_{44}^{(\text{eff})}$ is different, and tends to zero at the new band edge as expected. The non-zero k_x leads to non-zero $c_{45}^{(\text{eff})}$, and the parameter $c_{55}^{(\text{eff})}$ becomes complex-valued at the $k_x = 0$ band edge. Only the real parts of the quantities are shown in both figures. No attempt is made here to discuss their imaginary components, which requires careful analysis of the branch cuts and is a topic for separate study.

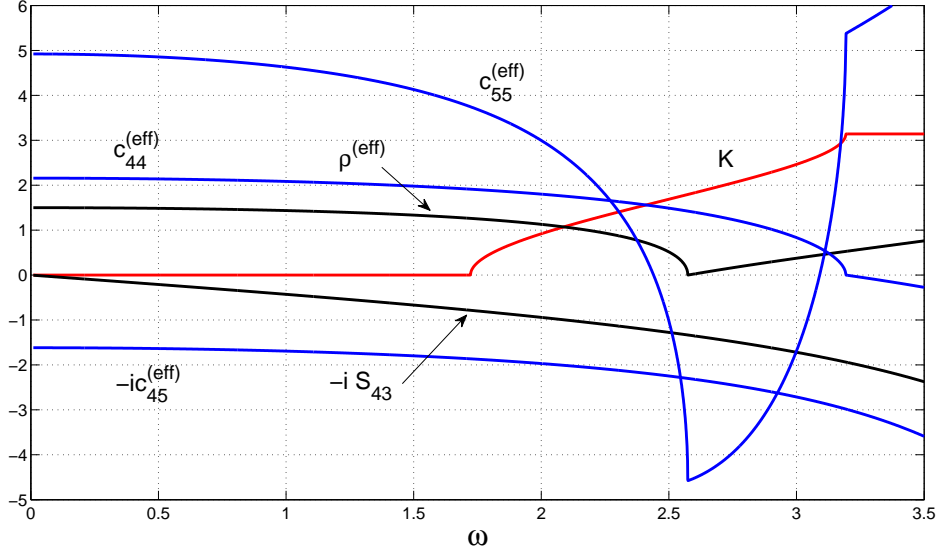


Figure 2: The same as in Figure 1 but for $k_x = 1.0$. The additional parameters $c_{55}^{(\text{eff})}$ and $c_{45}^{(\text{eff})}$ are relevant to $k_x \neq 0$. Only the real parts of the quantities are plotted.

4.3.2 Reflection and transmission of a half-space of effective material

As an example of the type of boundary problem that can be solved using the effective medium equations, consider reflection-transmission of SH waves at a bonded interface $y = 0$ between the half-space of the periodically stratified medium ($y > 0$) and a uniform half-space ($y < 0$) of isotropic material with ρ_0 , μ_0 and $c_0 = \sqrt{\mu_0/\rho_0}$. A SH plane wave is incident from the uniform half-space with propagation direction at angle θ from the interface normal. The total solution is taken as

$$u(x, y) = e^{ik_x x} \times \begin{cases} [e^{ik_y y} + R e^{-ik_y y}], & y \leq 0, \\ T e^{iK(\omega, k_x) y}, & y > 0, \end{cases} \quad \text{with } (k_x, k_y) = \frac{\omega}{c_0} (\sin \theta, \cos \theta). \quad (49)$$

The reflection and transmission coefficients R and T follow from the continuity conditions for particle velocity and traction at the interface. They may be expressed in standard form using SH impedances defined as $Z_{\pm} = -\sigma_{23}/\dot{u}|_{y=0_{\pm}}$. The impedance in the uniform half-space is $Z_- = \rho_0 c_0 \cos \theta$. The impedance Z_+ for the effective medium follows from (43) as

$$Z_+ = \omega^{-1} (K c_{44}^{(\text{eff})} + k_x c_{45}^{(\text{eff})} - \omega S_{43}). \quad (50)$$

This is identical to the impedance of the periodically stratified half-space because they both imply a ratio of components of the outgoing eigenvector \mathbf{w} which is common to $\mathbf{M}(T, 0)$ and \mathbf{K} . In these terms, the continuity conditions for displacement and traction yield the exact result

$$1 + R = T, \quad Z_-(1 - R) = Z_+ T, \quad \Rightarrow \quad R = \frac{Z_- - Z_+}{Z_- + Z_+}, \quad T = \frac{2Z_-}{Z_- + Z_+}. \quad (51)$$

Figure 3 shows $|R(\omega)|$ and $|T(\omega)|$ calculated for normal incidence from a uniform half-space with $\rho_1 = 1$, $c_1 = 1$ on a periodic structure of two layers with $\rho_1 = 1$, $c_1 = 1$, $\rho_2 = 2$, $c_2 = 2$, which was used in Figs. 1 and 2. As expected, $|R| \leq 1$ with total reflection in the stopband.

The explicit dependence of the reflection coefficient on the effective medium parameters $c_{44}^{(\text{eff})}$, $c_{45}^{(\text{eff})}$ and S_{43} means that, in principle, measurement of R via experiment can provide useful knowledge for their determination.

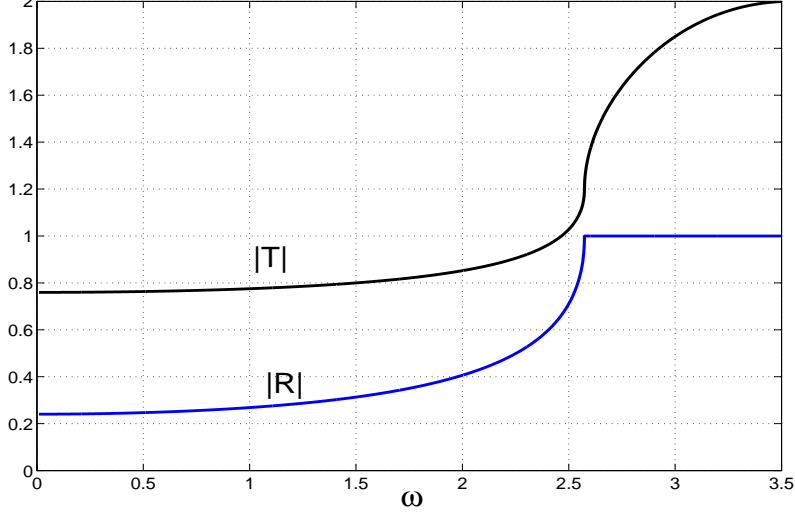


Figure 3: The magnitude of the reflection and transmission coefficients of (51) for normal incidence ($\theta = 0$).

4.3.3 Uniform normal impedance

It is instructive to consider the particular case of $k_x = 0$ with $z = \sqrt{\rho(y)\mu(y)} = \rho(y)c(y)$ independent of y , i.e. $z \equiv z_0$. The 2×2 matrix $\mathbf{Q}(y)$ is then a scalar multiple of a constant matrix, and $M_1(0) = M_4(0)$, $M_2(0) = (i\omega z_0)^{-1} \sin KT$ (where (0) stands for $k_x = 0$). As a result, by (46), the effective parameters at any ω retain their values obtained from static averaging: $S_{43} = 0$, $c_{44}^{(\text{eff})}(\omega, 0) = \langle \mu^{-1} \rangle^{-1}$ and $\rho^{(\text{eff})}(\omega) = \langle \rho \rangle$. This simplification is a consequence of the fact that constant z implies constant eigenvectors of the SH matricant $\mathbf{M}(y, 0)$ and hence no reflection of SH waves normally propagating through a periodic structure, which is in accordance with the physical meaning of the impedance z . Consistency is also observed in that the effective impedance $z^{(\text{eff})}$ defined through the above effective parameters is equal to z_0 ,

$$z^{(\text{eff})} = \sqrt{\rho^{(\text{eff})} c_{44}^{(\text{eff})}} = \rho^{(\text{eff})} c^{(\text{eff})} = \sqrt{\langle \rho \rangle \langle \mu^{-1} \rangle^{-1}} = z_0. \quad (52)$$

The only effect of the inhomogeneity is to speed up or retard advancing waves according to the effective speed $c^{(\text{eff})} = z^{(\text{eff})}/\rho^{(\text{eff})}$, which in the present case follows from (52) as $c^{(\text{eff})} = z_0/\rho^{(\text{eff})} = \langle c^{-1} \rangle^{-1}$.

4.3.4 Discussion

In the case of purely uni-dimensional motion, $k_x = 0$, the system (43) involves only the first three parameters of Eq. (47): $c_{44}^{(\text{eff})}$, $\rho^{(\text{eff})}$, and S_{43} . Willis [14] derived expressions for the same quantities for a laminated medium. His coefficients [14, Eq. (3.30)] relate weighted means of strain and

velocity ($\langle we \rangle$, $\langle wi \rangle$) to ensemble means of stress and momentum density ($\langle \sigma \rangle$, $\langle p \rangle$), where w is a general weighting function first introduced in [13], such that ensemble means correspond to $w = 1$. The Willis parameters derived here, e.g. (43), concern strain and velocity at the single point $y = 0$ in the unit period, and therefore correspond to the specific weight function $w(x) = 2L\delta(x)$ in the notation of [14]. It is important to note, however, that the stress and momentum density used here are not ensemble averages but are quantities associated with the same point in the unit period. This identification, for instance, means that the solution of the reflection-transmission problem of §4.3.2 is in fact the deterministic solution. In summary, while the governing equations are the same in both cases, the Willis parameters developed here do not bear a one-to-one correspondence with those in [14].

5 Conclusion

A fully dynamic homogenization scheme has been developed for periodically layered anisotropic elastic solids. In the process, the dispersive and nonlocal Willis model has been shown to provide an optimal constitutive setting for the effective medium. The crucial point of the present method is the insistence that the matrix of coefficients \mathbf{Q}_{eff} of the sextic system of elastodynamics equations, for whatever homogeneous effective medium is considered, must exactly match the Floquet wave number matrix \mathbf{K} of the periodic system. This is not a low-frequency long-wave approach, so long as \mathbf{K} is defined at the given frequency ω and horizontal wave number k_x . The wave number matrix $\mathbf{K} = \mathbf{K}(\omega, k_x)$ is an analytic function of ω and k_x that may be explicitly defined via the Magnus series expansion, which is guaranteed to converge below the first Floquet stopband at the edge of the Brillouin zone. The choice of constitutive model for the effective medium is critical. We have demonstrated that the standard anisotropic elasticity theory does not suffice as it cannot provide a \mathbf{Q}_{eff} to properly account for dynamic terms appearing in the wave number matrix $\mathbf{K}(\omega, k_x)$. On the other hand, the Willis model for the effective medium, which includes coupling effects, can allow us to associate elements of the effective system matrix \mathbf{Q}_{eff} with elements in \mathbf{K} . The main results are contained in Eqs. (23) and (26) which infer the material parameters of the effective Willis medium from \mathbf{K} . Invoking the Magnus series, explicit expressions for the low-frequency long-wave expansion of these effective Willis parameters have been found and the accuracy for their truncated asymptotics has been estimated.

The example of SH plane wave reflection and transmission considered in §4.3.2 indicates the type of application possible using the Willis effective medium. The point is not so much to provide new solutions for layered media, although it is simpler to formulate and solve such problems using equations for a homogeneous model. The potential power of the dynamic effective medium model is that it is possible to relate the effective properties of the Willis material to measurable dynamic quantities. Thus, the reflection and transmission problem illustrates how the reflection coefficient R depends on a certain combination of the Willis parameters. Measurements of $R = R(\omega, k_x)$ provide a means to characterize periodic layered systems as equivalent homogeneous but dispersive materials. Other problems that may be considered are, for instance, surface wave propagation in a periodically layered half space, waveguides comprised of periodic layers, and point forces.

Acknowledgements

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Appendix

A. Estimates for the long-wavelength expansion of \mathbf{K}

A.1 Auxiliary notations

For any $2d \times 2d$ matrix \mathbf{A} consisting of $d \times d$ blocks \mathbf{A}_J ($J = 1, \dots, 4$), denote a 2×2 matrix of matrix norms $\|\mathbf{A}_J\|$ by $\|\mathbf{A}\|_{2 \times 2}$:

$$\|\mathbf{A}\|_{2 \times 2} = \begin{pmatrix} \|\mathbf{A}_1\| & \|\mathbf{A}_2\| \\ \|\mathbf{A}_3\| & \|\mathbf{A}_4\| \end{pmatrix}. \quad (53)$$

Note that $\|\mathbf{A}\mathbf{B}\|_{2 \times 2} \leq \|\mathbf{A}\|_{2 \times 2} \|\mathbf{B}\|_{2 \times 2}$, where and hereafter a matrix inequality is understood as that between the corresponding matrix elements. Let

$$\nu^2 = \langle N_1 \rangle^2 + \langle N_2 \rangle \langle N_3 \rangle, \quad q(y) = \max(\|\mathbf{N}_J(y)\| / \langle N_J \rangle, \rho(y) / \langle \rho \rangle), \quad (54)$$

where $\langle \cdot \rangle$ is the averaging symbol and $\langle N_J \rangle$ is an average of a norm $N_J(y) = \|\mathbf{N}_J(y)\|$ of the Stroh-matrix block ($J = 1, 2, 3$). ($\|\mathbf{N}_1\| = \|\mathbf{N}_4\|$). Both ν and $q(y)$ are physically dimensionless and strictly positive. The magnitude of ν is usually of the order of 1 unless a high-contrast case affecting the averaged profile; in turn, the averaged value $\langle q \rangle$, strictly speaking, satisfies $1 \leq \langle q \rangle \leq 4$ but is typically close to 1 as well. Let us define the long-wave small parameter ε as

$$\varepsilon \equiv kT \text{ with } k = \sqrt{k_x^2 + \omega^2/V^2}, \quad V^2 = (\langle N_1 \rangle^2 + \langle N_3 \rangle \langle N_2 \rangle) (\langle \rho \rangle \langle N_2 \rangle)^{-1}. \quad (55)$$

It is noted that $\epsilon = \nu\varepsilon$ may equally be taken as such a parameter and that it can actually be replaced everywhere below by a smaller value

$$\tilde{\varepsilon} = T \max(k_x \langle N_1 \rangle, k_x \sqrt{\langle N_2 \rangle \langle N_3 \rangle}, \omega \sqrt{\langle \rho \rangle \langle N_2 \rangle}) < \nu\varepsilon. \quad (56)$$

Next, define

$$\mathbf{C} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \frac{T \langle N_2 \rangle}{\nu\varepsilon} \mathbf{I} \end{pmatrix}, \quad \widehat{\mathbf{Q}}(y) = \mathbf{C} \mathbf{Q}(y) \mathbf{C}^{-1} = i \begin{pmatrix} k_x \mathbf{N}_1 & \frac{\nu\varepsilon}{T \langle N_2 \rangle} \mathbf{N}_2 \\ \frac{T \langle N_2 \rangle}{\nu\varepsilon} (k_x^2 \mathbf{N}_3 - \rho \omega^2) & k_x \mathbf{N}_1^T \end{pmatrix}, \quad (57)$$

where $\mathbf{Q}(y)$ is given in (3), and the normalization of $\widehat{\mathbf{Q}}(y)$ provides a common estimate $\|\widehat{\mathbf{Q}}_J(y)\| T \leq \nu\varepsilon q(y)$ for the blocks of $\widehat{\mathbf{Q}}$, from which follow the estimates for $\|\mathbf{Q}_J(y)\|$. Denoting the (constant) 2×2 matrices

$$\mathbf{H} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \|\mathbf{C}\|_{2 \times 2} \equiv \tilde{\mathbf{C}} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{\nu\varepsilon} T \langle N_2 \rangle \end{pmatrix}, \quad \mathbf{\Omega} = \frac{1}{T} \nu\varepsilon \langle q \rangle \tilde{\mathbf{C}}^{-1} \mathbf{H} \tilde{\mathbf{C}}, \quad (58)$$

and using the notation (53) enables us to write the blockwise estimates for $\widehat{\mathbf{Q}}(y)$ and for $\mathbf{Q}(y)$ in the form

$$\begin{aligned} \|\widehat{\mathbf{Q}}(y)\|_{2 \times 2} T \leq \nu\varepsilon q(y) \mathbf{H} &\Rightarrow \|\mathbf{Q}(y)\|_{2 \times 2} = \tilde{\mathbf{C}}^{-1} \|\widehat{\mathbf{Q}}(y)\|_{2 \times 2} \tilde{\mathbf{C}} \leq \frac{q(y)}{\langle q \rangle} \mathbf{\Omega} \\ &\Rightarrow \|\langle \mathbf{Q} \rangle\|_{2 \times 2} \leq \langle \|\mathbf{Q}\|_{2 \times 2} \rangle \leq \mathbf{\Omega}. \end{aligned} \quad (59)$$

Note the meaning of $\mathbf{\Omega}$ as a matrix of upper bounds of blocks of the statically averaged system matrix $\langle \mathbf{Q} \rangle$.

A.2 Estimates for the Magnus series $i\mathbf{K} = \sum_{m=0}^{\infty} i\mathbf{K}^{(m)}$

An elegant proof that the Magnus series (13) converges for $\langle \|\mathbf{Q}\|_2 \rangle T < \pi$ [16] is somewhat implicit in that it does not provide fully explicit estimates of the series terms and remainder. These may be obtained for a narrower range by adapting the derivation detailed and referenced in [11]. It proceeds from the estimate

$$\|\mathbf{K}^{(m)}\|_T \leq \pi (\xi T \langle \|\mathbf{Q}\| \rangle)^{m+1}, \quad \xi = 2 \left(\int_0^\pi [2 + x(1 - \cot x)]^{-1} dx \right)^{-1} = 1.8400... \quad (60)$$

with specifically the matrix norm $\|\cdot\|_2$ as kept tacit below. (Note aside that the physical dimension of $(\mathbf{Q}T)^n$ is the same for any n as that of $\mathbf{Q}T$ and $\mathbf{K}^{(m)}T$.) Let $i\widehat{\mathbf{K}} = \sum_{m=0}^{\infty} i\widehat{\mathbf{K}}^{(m)}$ be the same series (13) but related to the matrix $\widehat{\mathbf{Q}}$ in place of \mathbf{Q} . Applying (60) yields the blockwise estimates for series terms $\widehat{\mathbf{K}}^{(m)}$ and, hence, $\mathbf{K}^{(m)}$ in the form

$$\|\widehat{\mathbf{K}}^{(m)}\|_{2 \times 2} T \leq \pi X^{m+1} \mathbf{H} \Rightarrow \|\mathbf{K}^{(m)}\|_{2 \times 2} \leq \pi \xi X^m \mathbf{\Omega}, \quad \text{where } X = \xi \nu \varepsilon \langle q \rangle. \quad (61)$$

Assume hereafter that $X < 1$ (which is within the convergence radius $X < \xi \frac{\pi}{2}$ that follows from the result $\langle \|\mathbf{Q}\| \rangle T < \pi$ of [16]). By (61), the residual series $\widehat{\mathbf{R}}^{(M)} = \sum_{m=M}^{\infty} i\widehat{\mathbf{K}}^{(m)}$ and $\mathbf{R}^{(M)} = \sum_{m=M}^{\infty} i\mathbf{K}^{(m)}$ satisfy

$$\|\widehat{\mathbf{R}}^{(M)}\|_{2 \times 2} T \leq \pi(1 - X)^{-1} X^{M+1} \mathbf{H} \Rightarrow \|\mathbf{R}^{(M)}\|_{2 \times 2} \leq \pi \xi (1 - X)^{-1} X^M \mathbf{\Omega}, \quad (62)$$

so that they decrease as M grows and tend to zero as $M \rightarrow \infty$.

Knowing the upper bound of $\|\mathbf{R}^{(M)}\|_{2 \times 2}$ evaluates the sufficient number of terms to be kept in the Magnus series to ensure a desired accuracy of truncation for a fixed long-wave parameter ε , or else provides the value of ε that ensures this accuracy for a given truncation step. The accuracy is gauged by the matrix $\mathbf{\Omega}$ of blockwise bounds of $\langle \mathbf{Q} \rangle$, see (59). For example, let the Magnus series (13) be truncated as $i\mathbf{K} = \langle \mathbf{Q} \rangle + i\mathbf{K}^{(1)} + i\mathbf{K}^{(2)}$ and the remainder $\mathbf{R}^{(3)}$ discarded. According to (62)₂, $\|\mathbf{R}^{(3)}\|_{2 \times 2} \leq 5.8X^3 / (1 - X)$. Thus taking the spectral range as $\nu \varepsilon \langle q \rangle < 0.24$ or < 0.128 ensures $\|\mathbf{R}^{(3)}\|_{2 \times 2} < \mathbf{\Omega}$ or $< 0.1\mathbf{\Omega}$, respectively (note that truncating $i\mathbf{K}$ by $\langle \mathbf{Q} \rangle$ at $\nu \varepsilon \langle q \rangle < 0.128$ discards $\|\mathbf{R}^{(1)}\|_{2 \times 2} < 1.79\mathbf{\Omega}$).

It is noted that the above mentioned sufficient criterion for the Magnus series convergence and the bounds for its terms restrict ω and k_x by imposing conditions on the norm $\|\mathbf{Q}\|$ of $\mathbf{Q} = \mathbf{Q}(y; \omega, k_x)$. At the same time, if \mathbf{Q} is independent of y then the Magnus series certainly converges at any ω and k_x . Hence if the inhomogeneity is relatively weak so that $\|\mathbf{Q} - \langle \mathbf{Q} \rangle\|$ is markedly smaller than $\|\mathbf{Q}\|$, then the ω and k_x bounds on the Magnus series can be eased by using a different approach that is based, instead of (60), on the estimate $\|\mathbf{K}^{(m)}\| \leq Cm \langle \|\mathbf{Q} - \langle \mathbf{Q} \rangle\| \rangle^m$ ($C > 0$ is some constant). The latter acquires a growing factor m but is hinged explicitly on $\|\mathbf{Q} - \langle \mathbf{Q} \rangle\|$, which is why this approach can be much more advantageous for small $\|\mathbf{Q} - \langle \mathbf{Q} \rangle\|$.

A.3 Invertibility of \mathbf{K}_2

Derivation of the effective material constants requires inverting the block \mathbf{K}_2 (see §3.2). Evidently $i\mathbf{K}_2 = i\langle \mathbf{N}_2 \rangle + \mathbf{R}_2^{(1)}$ is assuredly negative definite (like $\langle \mathbf{N}_2 \rangle$) if $\|\langle \mathbf{N}_2 \rangle^{-1} \mathbf{R}_2^{(1)}\| < 1$. Inserting $\|\mathbf{R}_2^{(1)}\| \leq \pi \xi \langle q \rangle \langle N_2 \rangle X / (1 - X)$ from (62)₂ and resolving the resulting inequality with respect to $\nu \varepsilon \langle q \rangle$ yields

$$\nu \varepsilon \langle q \rangle < \left(2 + 11 \langle q \rangle \langle N_2 \rangle \|\langle \mathbf{N}_2 \rangle^{-1}\| \right)^{-1}. \quad (63)$$

This condition can be further improved by using more precise estimates for the low-order terms of the Magnus series. For this purpose, it is suitable to proceed from $\widehat{\mathbf{K}}^{(m)}$ defined by (13) with $\widehat{\mathbf{Q}}$. Using $\int_0^1 \dots \int_0^{\tilde{\zeta}_{m-1}} q(\tilde{\zeta}) \dots q(\tilde{\zeta}_m) \mathbf{H}^m = \frac{2^{m-1} \langle q \rangle^m}{m!} \mathbf{H}$ and $\|\mathbf{K}_2^{(m)}\| = \frac{T \langle N_2 \rangle}{\nu \varepsilon} \|\widehat{\mathbf{K}}_2^{(m)}\|$ gives for $m = 1, 2$:

$$\begin{aligned} \|\widehat{\mathbf{K}}^{(1)}\|_{2 \times 2} T &\leq \frac{(2\nu\varepsilon\langle q \rangle)^2}{4} \mathbf{H}, \quad \|\widehat{\mathbf{K}}^{(2)}\|_{2 \times 2} T \leq \frac{(2\nu\varepsilon\langle q \rangle)^3}{9} \mathbf{H} \Rightarrow \\ \|\mathbf{K}_2^{(1)}\| &\leq \nu\varepsilon \langle q \rangle \langle N_2 \rangle, \quad \|\mathbf{K}_2^{(2)}\| \leq \frac{4}{9} \nu\varepsilon \langle q \rangle^2 \langle N_2 \rangle, \end{aligned} \quad (64)$$

where the right-hand sides are smaller than in (61) with $m = 1, 2$. Exploiting (64) leads to

$$\begin{aligned} \|\langle \mathbf{N}_2 \rangle^{-1} \mathbf{R}_2^{(1)}\| &= \|\langle \mathbf{N}_2 \rangle^{-1} \left(\sum_{m=1}^2 i \mathbf{K}_2^{(m)} + \mathbf{R}^{(3)} \right)\| \\ &\leq 2 \langle q \rangle \langle N_2 \rangle \|\langle \mathbf{N}_2 \rangle^{-1}\| \left(0.272X + 0.132X^2 + 2.93X^3 / (1 - X) \right) \\ \Rightarrow \|\langle \mathbf{N}_2 \rangle^{-1} \mathbf{R}_2^{(1)}\| &< 1 \text{ if } X < \min \left(0.41, (1 + 1.4 \langle q \rangle \langle N_2 \rangle \|\langle \mathbf{N}_2 \rangle^{-1}\|)^{-1} \right). \end{aligned} \quad (65)$$

Hence, by (65), taking a typical value $\langle q \rangle \langle N_2 \rangle \|\langle \mathbf{N}_2 \rangle^{-1}\| \approx 1$ guarantees that \mathbf{K}_2 is invertible in the spectral range $X < 0.41$, i.e. $\nu\varepsilon \langle q \rangle < 0.22$.

A.4 Estimate for the eigenvalues of \mathbf{K}

The upper bound for eigenvalues K_α of \mathbf{K} may be evaluated via $\|K_\alpha\| \leq \|\mathbf{K}\|$; however, taking note that K_α are also the eigenvalues of $\widehat{\mathbf{K}}$ yields a better estimate with regard for $(62)_1$ as follows

$$\|K_\alpha\| \leq \|\widehat{\mathbf{K}}\| = \|\widehat{\mathbf{R}}^{(0)}\| \leq 2\|\widehat{\mathbf{R}}^{(0)}\|_{2 \times 2} \leq 2\pi T^{-1} (1 - X)^{-1} X \quad (66)$$

(note that K_α here may certainly take either real or complex values). For instance, $\|K_\alpha\|T < 0.62$ in the long-wave range $\nu\varepsilon \langle q \rangle < 0.128$ ($X < 0.236$) that was shown in §A.2 to ensure accuracy of truncation of \mathbf{K} after $\mathbf{K}^{(2)}$. Note that vanishing of the right-hand side of (66) at $X = 0$, i.e. at $\varepsilon = T\sqrt{k_x^2 + \omega^2/V^2} = 0$ (see (55)) is in agreement with $\mathbf{K} = \begin{pmatrix} \mathbf{0} & \langle \mathbf{N}_2 \rangle \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$ at $\omega = 0$, $k_x = 0$.

A.5 Convergence of $\partial\mathbf{K}/\partial k_x$

Consider $(\partial\mathbf{K}/\partial k_x)_{k_x=0} \equiv \mathbf{K}'(0)$ as defined by Eq. (29). The series (28₁) and (29₁) assuredly converge if so does the same series for $\ln \mathbf{CMC}^{-1} = \mathbf{C}(\ln \mathbf{M})\mathbf{C}^{-1}$, where \mathbf{C} is introduced in (57₁). In turn the series for $\ln \mathbf{CMC}^{-1}$ assuredly converges if

$$\|\mathbf{CMC}^{-1} - \mathbf{I}\| \leq \|\exp\langle \|\widehat{\mathbf{Q}}\| \rangle - \mathbf{I}\| \leq \exp(2\nu\varepsilon \langle q \rangle) - 1 < 1 \Rightarrow 2\nu\varepsilon \langle q \rangle < \ln 2, \quad (67)$$

where it was used that $\|\widehat{\mathbf{Q}}\| = 2\nu\varepsilon \langle q \rangle$ due to (59₁) and $\|\mathbf{H}\| = 2$. For $\mathbf{M} \equiv \mathbf{M}(0)$ with $k_x = 0$, which is the case in hand, the condition (67) reduces, using (56), to

$$2\tilde{\varepsilon}(0) \langle q(0) \rangle < \ln 2, \quad (68)$$

where $\tilde{\varepsilon}(0) = T \max(\omega\sqrt{\langle \rho \rangle \langle N_2 \rangle})$, $q(0) = \max(\|\mathbf{N}_2(y)\|/\langle N_2 \rangle, \rho(y)/\langle \rho \rangle)$ ($1 \leq \langle q(0) \rangle \leq 2$).

The integrals in (28₂) and (29₂) exist provided the matrix $\mathbf{I} + x(\mathbf{M}(0) - \mathbf{I})$ is invertible for any $x \in (0, 1)$. According to [16], this is guaranteed if

$$2\tilde{\varepsilon}(0) \langle q(0) \rangle < \pi, \quad (69)$$

which implies that the eigenvalues $e^{iK_\alpha(0)T}$ of $\mathbf{M}(0)$ do not attain real negative values. This condition coincides with the sufficient condition for the convergence of Magnus series at $k_x = 0$.

B. Effective medium coefficients for SH waves at long wavelength

According to (13) truncated by $\mathbf{K}^{(2)}$,

$$\mathbf{Q}_{\text{eff}} = i \begin{pmatrix} K_1^{(1)} & -\langle \mu^{-1} \rangle + K_2^{(2)} \\ \langle \mu \rangle k_x^2 - \langle \rho \rangle \omega^2 + K_3^{(2)} & -K_1^{(1)} \end{pmatrix}, \quad (70)$$

where $K_{2,3}^{(1)} = 0$, $K_1^{(2)} = 0$ and (omitting the integration variables)

$$\begin{aligned} K_1^{(1)} &= \frac{iT}{2} \int_0^1 \int_0^{\tilde{\zeta}} [\mu^{-1}, \rho\omega^2 - \mu k_x^2], \\ \{K_2^{(2)}, K_3^{(2)}\} &= \frac{T^2}{3} \int_0^1 \int_0^{\tilde{\zeta}} \int_0^{\tilde{\zeta}_1} \{ [\mu^{-1}, [\rho\omega^2 - \mu k_x^2, \mu^{-1}]], [\rho\omega^2 - \mu k_x^2, [\mu^{-1}, \rho\omega^2 - \mu k_x^2]] \}. \end{aligned} \quad (71)$$

On the other hand, Eq. (45) taken to the same order as (70) and written with Voigt index notation, yields

$$\mathbf{Q}_{\text{eff}} = i \begin{pmatrix} -\langle \mu^{-1} \rangle (k_x c_{45}^{(1)} - \omega S_{43}^{(1)}) & -\langle \mu^{-1} \rangle + c_{44}^{(2)} \langle \mu^{-1} \rangle^2 \\ k_x^2 (\langle \mu \rangle + c_{55}^{(2)}) - \omega^2 (\langle \rho \rangle + \rho^{(2)}) & \langle \mu^{-1} \rangle (k_x c_{45}^{(1)} - \omega S_{43}^{(1)}) \\ + \langle \mu^{-1} \rangle (k_x c_{45}^{(1)} - \omega S_{43}^{(1)})^2 & \end{pmatrix}, \quad (72)$$

where $c_{45}^{(1)+} = c_{54}^{(1)} = -c_{45}^{(1)}$ has been used, and in addition $c_{44}^{(0)} = \langle \mu^{-1} \rangle^{-1}$, $c_{55}^{(0)} = \langle \mu \rangle$, $c_{44}^{(1)} = c_{55}^{(1)} = 0$, $\rho^{(1)} = 0$ with, as noted earlier, $S_{53}^{(1)} = 0$. From (70)-(72),

$$\begin{aligned} c_{45}^{(1)} &= \frac{i}{2} k_x T \langle \mu^{-1} \rangle^{-1} \int_0^1 \int_0^{\tilde{\zeta}} [\mu^{-1}, \mu], \quad S_{43}^{(1)} = \frac{i}{2} \omega T \langle \mu^{-1} \rangle^{-1} \int_0^1 \int_0^{\tilde{\zeta}} [\mu^{-1}, \rho], \\ c_{44}^{(2)} &= \langle \mu^{-1} \rangle^{-2} K_2^{(2)}, \quad k_x^2 c_{55}^{(2)} - \rho^{(2)} \omega^2 = K_3^{(2)} - \langle \mu^{-1} \rangle^{-1} K_1^{(1)2}, \end{aligned} \quad (73)$$

which identifies $c_{45}^{(1)}(k_x) = -c_{54}^{(1)}(k_x)$, $c_{44}^{(2)}(\omega^2, k_x^2)$ and $S_{43}^{(1)}(\omega)$. The density correction $\rho^{(2)}(\omega)$ follows from the final identity as equal to the expression (38)₁ with $c_{33} \rightarrow \mu$, and $c_{55}^{(2)}(\omega^2, k_x^2)$ is then uniquely defined. Similar results follow for the SH waves in a monoclinic periodic medium.

Note that the secular equation of the SH-wave matrix \mathbf{Q}_{eff} given by (70) can equally be associated, up to the same order as \mathbf{Q}_{eff} itself, with other matrices such as, e.g., the matrix

$$\tilde{\mathbf{Q}}_{\text{eff}} = i \begin{pmatrix} 0 & -\langle \mu^{-1} \rangle + K_2^{(2)} \\ \langle \mu \rangle k_x^2 - \langle \rho \rangle \omega^2 + K_3^{(2)} - \langle \mu^{-1} \rangle^{-1} K_1^{(1)2} & 0 \end{pmatrix}, \quad (74)$$

which has zero diagonal components like in (41) and thus leads to Eqs. (43), (73) but with zero $c_{45}^{(1)}$ and $S_{43}^{(1)}$. However, as remarked in §3.3.3, the effective polarization of the SH displacement-traction eigenmodes is asymptotically defined by the eigenvectors $\mathbf{w}_{1,2}$ of (truncated) $\mathbf{Q}_{\text{eff}} = i\mathbf{K}$, while its definition from the eigenvectors $\tilde{\mathbf{w}}_{1,2}$ of $\tilde{\mathbf{Q}}_{\text{eff}}$ is different since $\tilde{\mathbf{w}}_{1,2} \neq \mathbf{w}_{1,2}$ to the first order in ε .

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