Invited Paper

Homogenized dynamic constitutive relation for Bloch-wave propagation in periodic composites: structure and symmetries

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ABSTRACT

Central to the idea of metamaterials is the concept of dynamic homogenization which seeks to define frequency dependent effective properties for Bloch wave propagation. While the theory of static effective property calculations goes back about 60 years, progress in the actual calculation of dynamic effective properties for periodic composites has been made only very recently. Here we discuss the explicit form of the effective dynamic constitutive equations. We elaborate upon the existence and emergence of coupling in the dynamic constitutive relation and further symmetries of the effective tensors.

Keywords: Dynamic homogenization, Effective properties, Metamaterials

1. INTRODUCTION

Recent interest in the character of the overall dynamic properties of composites with tailored microstructure necessitates a systematic homogenization procedure to express the dynamic response of an elastic composite in terms of its average effective compliance and density. The elastostatic response of composites has been long understood to be non-local in space (Refs.[1–4]) but in the context of inhomogeneous elastodynamics, the effective constitutive relations are non-local in both space and time (Refs.[5,6]). Homogenization for calculating these overall dynamic properties of composites, based on the integration of the field variables, has been proposed by a number of researchers. For electromagnetic waves, see, for example Refs.[7–10] For elastodynamic waves Willis[11] has presented a homogenization method based on an ensemble averaging technique of the 'Bloch' reduced form of the wave propagating in a periodic composite; see also Refs.[12,13]

In the present paper we discuss the explicit form of the effective dynamic constitutive equations. We elaborate upon the existence and emergence of coupling in the dynamic constitutive relation and its dependence upon the architectural symmetries of the unit cell. We show that the averaged dynamic constitutive parameters are tensorial in nature and that the average strain tensor is coupled with the average momentum tensor. Such a form of the averaged constitutive relation where the constitutive parameters (including mass density) are tensors and where the average strain (average stress) is coupled with average linear momentum has been predicted in the literature (Refs.[11,13–15] and references cited therein). In general, the effective properties for the dynamic problem are not uniquely determined but they become unique in the presence of incompatible strains (Ref.[12]).

2. DYNAMIC HOMOGENIZATION

We express the solution to the elastodynamic equations of motion as the sum of the volume average and an additional deviation field due to the heterogeneous composition of the unit cell:

$$\hat{\mathbf{Q}} = \mathbf{Q}^0 + \mathbf{Q}^d \tag{1}$$

The aim is to derive a set of constitutive relations for the overall averaged parts of the field variables, using the local elastodynamic equations of motion and constitutive relations. This then provides the homogenized frequency-dependent material parameters.

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Consider harmonic waves in an unbounded elastic composite consisting of a collection of bonded, identical unit cells ($\Omega = \{x_i : -a_i/2 \leq x_i < a_i/2;\ i = 1,2,3\}$) which repeat themselves in all directions, and hence constitute a periodic structure. In view of the periodicity of the composite, we have $\rho(\mathbf{x}) = \rho(\mathbf{x} + m'\mathbf{I}_\beta)$ and $\mathbf{C}(\mathbf{x}) = \mathbf{C}(\mathbf{x} + m'\mathbf{I}_\beta)$; here m' is an integer, $\rho(\mathbf{x})$ is the density, $\mathbf{C}(\mathbf{x})$ is the fourth-order tensor of the modulus of elasticity whose inverse is the compliance tensor $\mathbf{D}(\mathbf{x})$, and $\mathbf{I}_\beta, \beta = 1,2,3$ denote the three vectors which form a parallelepiped enclosing the periodic unit cell. For time harmonic waves with frequency ω, the field quantities are proportional to $e^{\pm i\omega t}$. For waves with wave vector $\mathbf{q} = q_i\mathbf{e}_\mathrm{i}$ where $\mathbf{e}_\mathrm{i}$ is the unit vector in the i^{th} direction and the Einstein summation convention applies, the Bloch representation of the field variables takes the following form:

$$\hat{\mathbf{Q}}(\mathbf{x}, t) = \mathrm{Re}\left[\mathbf{Q}(\mathbf{x}) \exp[i(\mathbf{q} \cdot \mathbf{x} - \omega t)]\right] \tag{2}$$

where $\hat{\mathbf{Q}}$ represents the field variables, stress ($\hat{\boldsymbol{\sigma}}$), strain ($\hat{\boldsymbol{\varepsilon}}$), momentum ($\hat{\mathbf{p}}$) or velocity ($\hat{\dot{u}}$), whereas $\mathbf{Q}$ represents their periodic parts ($\boldsymbol{\sigma}$, $\boldsymbol{\varepsilon}$, $\mathbf{p}$, $\dot{\mathbf{u}}$). The representation, equation (2), separates the time harmonic and macroscopic factor from the microscopic part of the field variables. We emphasize here that the frequency and the wavevector, ω and $\mathbf{q}$, are, at this point, unrelated and arbitrary. Indeed, with $\mathbf{q}$ equal to zero and ω prescribed, the corresponding dynamic effective properties are obtained.

The local conservation and kinematic relations are

$$\begin{aligned} &\tilde{\nabla} \cdot \boldsymbol{\sigma} = -i\omega\mathbf{p} \\ &(\tilde{\nabla} \otimes \dot{\mathbf{u}})_{sym} = -i\omega\boldsymbol{\varepsilon} \end{aligned} \tag{3}$$

where $\tilde{\nabla} \to \nabla + i\mathbf{q}$. The corresponding local constitutive relations are

$$\begin{aligned} &\boldsymbol{\varepsilon} = \mathbf{D} : \boldsymbol{\sigma} \\ &\mathbf{p} = \rho\dot{\mathbf{u}} \end{aligned} \tag{4}$$

where $\mathbf{D}(\mathbf{x}) = \mathbf{C}(\mathbf{x})^{-1}$ is the tensor of compliance and $\rho(\mathbf{x})$ is the density of the material. These local material parameters represent the structure and composition of the unit cell.

Now we replace the heterogeneous unit cell with a homogeneous one having a suitable positive uniform density ρ^0 and a positive-definite compliance $\mathbf{D}^0 = [\mathbf{C}^0]^{-1}$ with the usual symmetries. These reference material parameters can be chosen for convenience without affecting the final overall average properties. In order to reproduce the strain and momentum of the actual unit cell, field variables eigenstrain, $\mathbf{E}(\mathbf{x})$, and eigenmomentum, $\mathbf{P}(\mathbf{x})$, are introduced. These quantities are then calculated, using the basic local field equations and constitutive relations. The idea stems from the polarization stress or strain that was originally proposed by[16] and further developed by,[17–19] and later by others, in order to construct energy-based bounds for the composite's overall elastic moduli. The basic tool in these works has been the result, obtained by[20] in three dimensions and earlier by[21] in two dimensions, that the stress and strain are constant within an ellipsoidal (elliptical in two dimensions) region of an infinitely extended uniform elastic medium when that region undergoes a uniform transformation corresponding to a uniform inelastic strain.

we require that the actual values of the field variables at every point within the homogenized and the original heterogeneous unit cell be exactly the same. To ensure this, we require that the following *consistency conditions* hold at every point within the unit cell ($\mathbf{x}$ dependence implicit in all field variables and eigenfields):

$$\begin{aligned} &\boldsymbol{\varepsilon} = \mathbf{D}^0 : \boldsymbol{\sigma} - \mathbf{E} \\ &\mathbf{p} = \rho^0\dot{\mathbf{u}} - \mathbf{P} \end{aligned} \tag{5}$$

The eigenstrain and eigenmomentum fields are zero in regions where the material properties of the heterogeneous unit cell are equal to the chosen uniform material properties $\mathbf{D}^0$ and ρ^0. From equations (3,5) we have

$$\tilde{\nabla} \cdot \mathbf{C}^0 : (\tilde{\nabla} \otimes \dot{\mathbf{u}})_{sym} + \omega^2\rho^0\dot{\mathbf{u}} = \omega^2\mathbf{P} + i\omega(\tilde{\nabla} \cdot \mathbf{C}^0 : \mathbf{E}) \tag{6}$$

$$\mathbf{C}^0 : [\tilde{\nabla} \otimes (\tilde{\nabla} \cdot \boldsymbol{\sigma})]_{sym} + \omega^2\rho^0\boldsymbol{\sigma} = \omega^2\rho^0\mathbf{C}^0 : \mathbf{E} + i\omega\mathbf{C}^0 : (\tilde{\nabla} \otimes \mathbf{P})_{sym} \tag{7}$$

Since the stress and displacement fields ($\mathbf{Q}$) are periodic (also for an RVE, viewed as a unit cell), they can be expanded in a spatial Fourier series:

$$\mathbf{Q}(\mathbf{x}) = \langle \mathbf{Q} \rangle + \mathbf{Q}^p = \langle \mathbf{Q} \rangle + \sum_{\boldsymbol{\xi} \neq 0} \mathbf{Q}(\boldsymbol{\xi}) \mathrm{e}^{i\boldsymbol{\xi} \cdot \mathbf{x}} \tag{8}$$

$$\langle \mathbf{Q} \rangle = \frac{1}{\Omega} \int_{\Omega} \mathbf{Q}(\mathbf{x}) dV_x \tag{9}$$

$$\mathbf{Q}(\boldsymbol{\xi}) = \frac{1}{\Omega} \int_{\Omega} \mathbf{Q}(\mathbf{x}) \mathrm{e}^{-i\boldsymbol{\xi} \cdot \mathbf{x}} dx \tag{10}$$

$$\Omega = 8a_1 a_2 a_3 \tag{11}$$

$$\boldsymbol{\xi} = \xi_i \mathbf{e}_{\mathrm{i}}; \quad \xi_\alpha = n_\alpha \pi / a_\alpha; \quad n_\alpha \text{ integers} \tag{12}$$

where Greek indices are not summed. In the above equations, $\langle \mathbf{Q} \rangle$ represents the averaged value of the field variable over the unit cell and appears in its macroscopic description, and $\mathbf{Q}^p(\mathbf{x})$, which is periodic with zero mean value, represents the local deviations from the average value.

Equations (6,7) become

$$-\boldsymbol{\zeta} \cdot \mathbf{C}^0 : (\boldsymbol{\zeta} \otimes \dot{\mathbf{u}})_{sym} + \omega^2 \rho^0 \dot{\mathbf{u}} = \omega^2 \mathbf{P} - \omega(\boldsymbol{\zeta} \cdot \mathbf{C}^0 : \mathbf{E}) \tag{13}$$

$$-\mathbf{C}^0 : [\boldsymbol{\zeta} \otimes (\boldsymbol{\zeta} \cdot \boldsymbol{\sigma})]_{sym} + \omega^2 \rho^0 \boldsymbol{\sigma} = \omega^2 \rho^0 \mathbf{C}^0 : \mathbf{E} - \omega \mathbf{C}^0 : (\boldsymbol{\zeta} \otimes \mathbf{P})_{sym} \tag{14}$$

where $\boldsymbol{\zeta} = \boldsymbol{\xi} + \mathbf{q}$. For the case of an isotropic reference material we have

$$C^0_{ijkl} = \lambda^0 \delta_{ij} \delta_{kl} + \mu^0 [\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}] \tag{15}$$

where λ^0 and μ^0 are the Lame$'$ constants. Using the isotropic stiffness tensor, the tensors in equations (13,14) can be inverted to give

$$\begin{aligned} \dot{\mathbf{u}}(\boldsymbol{\xi}) &= \boldsymbol{\Phi}(\boldsymbol{\zeta}) \cdot \mathbf{P}(\boldsymbol{\xi}) + \boldsymbol{\Theta}(\boldsymbol{\zeta}) : \mathbf{E}(\boldsymbol{\xi}) \\ \boldsymbol{\sigma}(\boldsymbol{\xi}) &= \boldsymbol{\Psi}(\boldsymbol{\zeta}) \cdot \mathbf{P}(\boldsymbol{\xi}) + \boldsymbol{\Gamma}(\boldsymbol{\zeta}) : \mathbf{E}(\boldsymbol{\xi}) \end{aligned} \tag{16}$$

where explicit expressions for tensors $\boldsymbol{\Phi}, \boldsymbol{\Theta}, \boldsymbol{\Psi}, \boldsymbol{\Gamma}$ are given in A. Now the stress and velocity fields can be expressed as a sum of their average and zero mean periodic components:

$$\dot{\mathbf{u}}(\mathbf{x}) = \langle \dot{\mathbf{u}} \rangle + \sum_{\boldsymbol{\xi} \neq 0} e^{i\boldsymbol{\xi} \cdot \mathbf{x}} \left[\boldsymbol{\Phi}(\boldsymbol{\zeta}) \cdot \frac{1}{\Omega} \int_{\Omega} \mathbf{P}(\mathbf{y}) e^{-i\boldsymbol{\xi} \cdot \mathbf{y}} dV_{\mathbf{y}} + \boldsymbol{\Theta}(\boldsymbol{\zeta}) : \frac{1}{\Omega} \int_{\Omega} \mathbf{E}(\mathbf{y}) e^{-i\boldsymbol{\xi} \cdot \mathbf{y}} dV_{\mathbf{y}} \right] \tag{17}$$

$$\boldsymbol{\sigma}(\mathbf{x}) = \langle \boldsymbol{\sigma} \rangle + \sum_{\boldsymbol{\xi} \neq 0} e^{i\boldsymbol{\xi} \cdot \mathbf{x}} \left[\boldsymbol{\Psi}(\boldsymbol{\zeta}) \cdot \frac{1}{\Omega} \int_{\Omega} \mathbf{P}(\mathbf{y}) e^{-i\boldsymbol{\xi} \cdot \mathbf{y}} dV_{\mathbf{y}} + \boldsymbol{\Gamma}(\boldsymbol{\zeta}) : \frac{1}{\Omega} \int_{\Omega} \mathbf{E}(\mathbf{y}) e^{-i\boldsymbol{\xi} \cdot \mathbf{y}} dV_{\mathbf{y}} \right] \tag{18}$$

where $\langle \dot{\mathbf{u}} \rangle$ and $\langle \boldsymbol{\sigma} \rangle$ are the average values of the velocity and stress fields, respectively, taken over a unit cell.

To make the homogenized unit cell point-wise equivalent to the original heterogeneous unit cell, the homogenizing fields are required to satisfy the following consistency conditions:

$$\boldsymbol{\epsilon}(\mathbf{x}) = \mathbf{D}(\mathbf{x}) : [\langle \boldsymbol{\sigma} \rangle + \boldsymbol{\sigma}^p] = \mathbf{D}^0 : [\langle \boldsymbol{\sigma} \rangle + \boldsymbol{\sigma}^p] - \mathbf{E} \tag{19}$$

$$\mathbf{p}(\mathbf{x}) = \rho(\mathbf{x}) [\langle \dot{\mathbf{u}} \rangle + \dot{\mathbf{u}}^p] = \rho^0 [\langle \dot{\mathbf{u}} \rangle + \dot{\mathbf{u}}^p] - \mathbf{P} \tag{20}$$

where $\mathbf{D}$ and $\mathbf{D}^0$ are the compliance tensors of the actual and the reference materials, respectively. The periodic parts of the velocity and stress fields, from equations (17,18), are now substituted into the above equations. This gives a set of 2 coupled integral equations which yields the required homogenizing stress and velocity fields that exactly and fully replace the heterogeneity in the original medium.

To obtain the overall effective properties, we only need to calculate the average quantities. To this end, average equations (19,20) over a unit cell (or an RVE) and obtain

$$\langle \boldsymbol{\epsilon} \rangle = \mathbf{D}^0 : \langle \boldsymbol{\sigma} \rangle - \langle \mathbf{E} \rangle \tag{21}$$

$$\langle \mathbf{p} \rangle = \rho^0 \langle \dot{\mathbf{u}} \rangle - \langle \mathbf{P} \rangle \tag{22}$$

To calculate $\langle \mathbf{E} \rangle$ and $\langle \mathbf{P} \rangle$, we divide the unit cell into $\bar{\alpha}$ subregions, Ω_α. Then we average the periodic fields over each such subregion to obtain

$$\begin{aligned} \langle \boldsymbol{\sigma}^p \rangle_{\Omega_\alpha} = \boldsymbol{\sigma}^{p\alpha} &= \frac{1}{\Omega_\alpha} \int_{\Omega_\alpha} \boldsymbol{\sigma}^p(\mathbf{x}) dV_{\mathbf{x}} \\ &= \sum_{\boldsymbol{\xi} \neq 0} g^\alpha(\boldsymbol{\xi}) \left[\boldsymbol{\Psi}(\boldsymbol{\zeta}) \cdot \frac{1}{\Omega} \int_\Omega \mathbf{P}(\mathbf{y}) e^{-i\boldsymbol{\xi}\cdot\mathbf{y}} dV_{\mathbf{y}} + \boldsymbol{\Gamma}(\boldsymbol{\zeta}) : \frac{1}{\Omega} \int_\Omega \mathbf{E}(\mathbf{y}) e^{-i\boldsymbol{\xi}\cdot\mathbf{y}} dV_{\mathbf{y}} \right] \end{aligned} \tag{23}$$

$$\begin{aligned} \langle \dot{\mathbf{u}}^p \rangle_{\Omega_\alpha} = \dot{\mathbf{u}}^{p\alpha} &= \frac{1}{\Omega_\alpha} \int_{\Omega_\alpha} \dot{\mathbf{u}}^p(\mathbf{x}) dV_{\mathbf{x}} \\ &= \sum_{\boldsymbol{\xi} \neq 0} g^\alpha(\boldsymbol{\xi}) \left[\boldsymbol{\Phi}(\boldsymbol{\zeta}) \cdot \frac{1}{\Omega} \int_\Omega \mathbf{P}(\mathbf{y}) e^{-i\boldsymbol{\xi}\cdot\mathbf{y}} dV_{\mathbf{y}} + \boldsymbol{\Theta}(\boldsymbol{\zeta}) : \frac{1}{\Omega} \int_\Omega \mathbf{E}(\mathbf{y}) e^{-i\boldsymbol{\xi}\cdot\mathbf{y}} dV_{\mathbf{y}} \right] \end{aligned} \tag{24}$$

$$g^\alpha(\boldsymbol{\xi}) = \frac{1}{\Omega_\alpha} \int_{\Omega_\alpha} \mathrm{e}^{i\boldsymbol{\xi}\cdot\mathbf{x}} dV_{\mathbf{x}} \tag{25}$$

We now replace the integrals in equations (23,24) by their equivalent finite sums and set

$$\begin{aligned} &\frac{1}{\Omega} \int_\Omega \mathbf{F}(\mathbf{y}) \mathrm{e}^{-i\boldsymbol{\xi}\cdot\mathbf{y}} dV_{\mathbf{y}} \approx \sum_\beta f^\beta g^\beta(-\boldsymbol{\xi}) \mathbf{F}^\beta \\ &f^\beta = \frac{\Omega_\beta}{\Omega} \\ &\mathbf{F}^\beta = \langle \mathbf{F} \rangle_{\Omega_\beta} \end{aligned} \tag{26}$$

Equations (23,24) then yield the following expressions:

$$\boldsymbol{\sigma}^{p\alpha} = \frac{1}{f^\alpha} \left[\boldsymbol{\Psi}^{\alpha\beta} \cdot \mathbf{P}^\beta + \boldsymbol{\Gamma}^{\alpha\beta} : \mathbf{E}^\beta \right] \tag{27}$$

$$\dot{\mathbf{u}}^{p\alpha} = \frac{1}{f^\alpha} \left[\boldsymbol{\Phi}^{\alpha\beta} \cdot \mathbf{P}^\beta + \boldsymbol{\Theta}^{\alpha\beta} : \mathbf{E}^\beta \right] \tag{28}$$

where the repeated index, β, is summed over the number of subregions, $\beta = 1, \ldots, \bar{\alpha}$, and Greek indices serve as labels for tensors rather than components of a particular tensor. The coefficient tensors in the above equations are defined by

$$\mathbf{M}^{\alpha\beta} = \sum_{\xi \neq 0} f^\alpha g^\alpha(\boldsymbol{\xi}) f^\beta g^\beta(-\boldsymbol{\xi}) \mathbf{M}(\boldsymbol{\zeta}) \tag{29}$$

In these equations, α and β are not summed. Averaging the consistency conditions over each subregion α and using equations (27,28), we have

$$\begin{aligned} &f^\alpha \langle \boldsymbol{\sigma} \rangle = -\bar{\boldsymbol{\Gamma}}^{\alpha\beta} : \mathbf{E}^\beta - \boldsymbol{\Psi}^{\alpha\beta} \cdot \mathbf{P}^\beta \quad \beta \textit{ summed} \\ &f^\alpha \langle \dot{\mathbf{u}} \rangle = -\boldsymbol{\Theta}^{\alpha\beta} : \mathbf{E}^\beta - \bar{\boldsymbol{\Phi}}^{\alpha\beta} \cdot \mathbf{P}^\beta \quad \beta \textit{ summed} \\ &\bar{\boldsymbol{\Gamma}}^{\alpha\beta} = \left[\boldsymbol{\Gamma}^{\alpha\beta} + \delta^{\alpha\beta} f^\alpha (\mathbf{D}^\alpha - \mathbf{D}^0)^{-1} : \mathbf{D}^0 \right] \\ &\bar{\boldsymbol{\Phi}}^{\alpha\beta} = \left[\boldsymbol{\Phi}^{\alpha\beta} + \mathbf{1}^{(2)} \tfrac{\rho^0}{\rho^\alpha - \rho^0} \delta^{\alpha\beta} f^\alpha \right] \end{aligned} \tag{30}$$

Equations (27,28) can now be inverted to express the eigenstrain tensors $\mathbf{E}^\beta$ and eigenmomentum tensors $\mathbf{P}^\beta$ in terms of the average stress $\langle\boldsymbol{\sigma}\rangle$ and average velocity $\langle\dot{\mathbf{u}}\rangle$ tensors. In addition, these piecewise constant eigenfields can be used to express the unit-cell-averaged eigenfields in terms of the average stress and average velocity tensors. The solution is formally written as

$$\begin{aligned}\langle\mathbf{E}\rangle &= \boldsymbol{\Delta} : \langle\boldsymbol{\sigma}\rangle + \boldsymbol{\Lambda}\cdot\langle\dot{\mathbf{u}}\rangle \\ \langle\mathbf{P}\rangle &= \boldsymbol{\Xi} : \langle\boldsymbol{\sigma}\rangle + \boldsymbol{\Omega}\cdot\langle\dot{\mathbf{u}}\rangle\end{aligned} \tag{31}$$

It should be stressed here that only the averages of the eigenfields are required for the determination of the effective properties. This, in turn, means that unlike the field integration method of[22] or,[7] the current formulation does not employ the pointwise elastodynamic solution. The formulation, however, is consistent with the elastodynamic problem, and the dispersion relation and the eigenvectors of the composite can be extracted from it (section 2.1). The averaged consistency conditions (21,22) are now expressed as

$$\langle\boldsymbol{\varepsilon}\rangle = \bar{\mathbf{D}} : \langle\boldsymbol{\sigma}\rangle + \bar{\mathbf{S}}_1\cdot\langle\dot{\mathbf{u}}\rangle \tag{32}$$

$$\langle\mathbf{p}\rangle = \bar{\mathbf{S}}_2 : \langle\boldsymbol{\sigma}\rangle + \bar{\boldsymbol{\rho}}\cdot\langle\dot{\mathbf{u}}\rangle \tag{33}$$

Equations (32,33) are our final constitutive relations for the homogenized composite.

3. MATHEMATICAL STRUCTURE OF THE CONSTITUTIVE RELATION

For each tensor $\mathbf{M}^{\alpha\beta}$ in equations (27,28) we have

$$\begin{aligned}\mathbf{M}^{\alpha\beta} &= \sum_{\xi>0}\left[f^\alpha g^\alpha(\boldsymbol{\xi})f^\beta g^\beta(-\boldsymbol{\xi})\mathbf{M}(\boldsymbol{\zeta}) + f^\alpha g^\alpha(-\boldsymbol{\xi})f^\beta g^\beta(\boldsymbol{\xi})\mathbf{M}(-\boldsymbol{\zeta})\right] \\ \mathbf{M}^{\beta\alpha} &= \sum_{\xi>0}\left[f^\beta g^\beta(\boldsymbol{\xi})f^\alpha g^\alpha(-\boldsymbol{\xi})\mathbf{M}(\boldsymbol{\zeta}) + f^\beta g^\beta(-\boldsymbol{\xi})f^\alpha g^\alpha(\boldsymbol{\xi})\mathbf{M}(-\boldsymbol{\zeta})\right] \\ \mathbf{M}^{\alpha\beta} &= \left[\mathbf{M}^{\beta\alpha}\right]^*\end{aligned} \tag{34}$$

This property also holds for tensors $\bar{\boldsymbol{\Gamma}}^{\alpha\beta}$ and $\bar{\boldsymbol{\Phi}}^{\alpha\beta}$. To facilitate inversion and solution, equations (30) are now expressed in their equivalent matrix form:

$$\begin{aligned}&\left[\mathbf{f}^1\right]\{\langle\boldsymbol{\sigma}\rangle\} = -\left[\boldsymbol{\Gamma}\right]\{\mathbf{E}\} - \left[\boldsymbol{\Psi}\right]\{\mathbf{P}\} \\ &\left[\mathbf{f}^2\right]\{\langle\dot{\mathbf{u}}\rangle\} = -\left[\boldsymbol{\Theta}\right]\{\mathbf{E}\} - \left[\boldsymbol{\Phi}\right]\{\mathbf{P}\} \\ &\{\langle\boldsymbol{\sigma}\rangle\}_{6(\alpha-1)+1}^{6(\alpha-1)+6} = \{\langle\sigma_{11}\rangle\ \langle\sigma_{22}\rangle\ \langle\sigma_{33}\rangle\ 2\langle\sigma_{23}\rangle\ 2\langle\sigma_{31}\rangle\ 2\langle\sigma_{12}\rangle\}^{\mathrm{T}} \\ &\{\langle\dot{\mathbf{u}}\rangle\}_{3(\alpha-1)+1}^{3(\alpha-1)+3} = \{\langle\dot{u}_1\rangle\ \langle\dot{u}_2\rangle\ \langle\dot{u}_3\rangle\}^{\mathrm{T}} \\ &\{\mathbf{E}\}_{6(\alpha-1)+1}^{6(\alpha-1)+6} = \{E_{11}^\alpha\ E_{22}^\alpha\ E_{33}^\alpha\ 2E_{23}^\alpha\ 2E_{31}^\alpha\ 2E_{12}^\alpha\}^{\mathrm{T}} \\ &\{\mathbf{P}\}_{3(\alpha-1)+1}^{3(\alpha-1)+3} = \{P_1^\alpha\ P_2^\alpha\ P_3^\alpha\}^{\mathrm{T}} \\ &\mathbf{f}_{ij}^1 = f^\alpha\delta_{ij};\quad \mathbf{f}_{kl}^2 = f^\alpha\delta_{kl} \\ &i = 6(\alpha-1)+1 : 6(\alpha-1)+6 \\ &j = 6(\alpha-1)+1 : 6(\alpha-1)+6 \\ &k = 3(\alpha-1)+1 : 3(\alpha-1)+3 \\ &l = 3(\alpha-1)+1 : 3(\alpha-1)+3 \\ &\alpha = 1 : \bar{\alpha}\end{aligned} \tag{35}$$

In the above equations $[\boldsymbol{\Gamma}]$ is a $6\bar{\alpha}\times 6\bar{\alpha}$ square matrix and $[\boldsymbol{\Phi}]$ is a $3\bar{\alpha}\times 3\bar{\alpha}$ square matrix. These matrices are composed of the components of the tensors $\bar{\boldsymbol{\Gamma}}^{\alpha\beta}$ and $\bar{\boldsymbol{\Phi}}^{\alpha\beta}$ appropriately placed at the matrix locations.

It can be shown that for any α and β we have

$$\begin{aligned}\left[\boldsymbol{\Gamma}\right]_{ij} &= \bar{\Gamma}_{pqrs}^{\alpha\beta} = \{\bar{\Gamma}_{pqrs}^{\beta\alpha}\}^* = \{\bar{\Gamma}_{rspq}^{\beta\alpha}\}^* = \left[\boldsymbol{\Gamma}\right]_{ji}^* \\ \left[\boldsymbol{\Phi}\right]_{ij} &= \bar{\Phi}_{pq}^{\alpha\beta} = \{\bar{\Phi}_{pq}^{\beta\alpha}\}^* = \{\bar{\Phi}_{qp}^{\beta\alpha}\}^* = \left[\boldsymbol{\Phi}\right]_{ji}^*\end{aligned} \tag{36}$$

where $\bar{\Gamma}^{\alpha\beta}_{pqrs}$, for instance, is the *pqrs* component of the tensor $\bar{\mathbf{\Gamma}}^{\alpha\beta}$. The above result signifies that the matrices $[\mathbf{\Gamma}]$ and $[\mathbf{\Phi}]$ are hermitian. We also note the following identity for the matrices $[\mathbf{\Psi}]$ and $[\mathbf{\Theta}]$:

$$[\mathbf{\Psi}]_{ij} = \Psi^{\alpha\beta}_{mnp} = \Theta^{\alpha\beta}_{pmn} = \{\Theta^{\beta\alpha}_{pmn}\}^* = [\mathbf{\Theta}]^*_{ji} \tag{37}$$

More generally, denoting a hermitian transpose by †, we have the following identities for the matrices:

$$\begin{aligned} &[\mathbf{\Gamma}]^\dagger = [\mathbf{\Gamma}] \\ &[\mathbf{\Phi}]^\dagger = [\mathbf{\Phi}] \\ &[\mathbf{\Psi}]^\dagger = [\mathbf{\Theta}]\,; \quad [\mathbf{\Theta}]^\dagger = [\mathbf{\Psi}] \end{aligned} \tag{38}$$

To expedite notation we omit the square brackets denoting a matrix in further calculations. *It must be stressed* that while unbracketed quantities in the main text represent tensors, they represent matrices in this appendix. This is done purely for the representational ease of the essential proofs which follow. We express the solution to equation (35) in the following form (matrix form of equation 31):

$$\begin{aligned} \mathbf{E} &= \mathbf{\Delta}\langle\boldsymbol{\sigma}\rangle + \mathbf{\Lambda}\langle\dot{\mathbf{u}}\rangle \\ \mathbf{P} &= \mathbf{\Xi}\langle\boldsymbol{\sigma}\rangle + \mathbf{\Omega}\langle\dot{\mathbf{u}}\rangle \end{aligned} \tag{39}$$

where

$$\begin{aligned} \mathbf{\Delta} &= \left[-\mathbf{\Gamma} + \mathbf{\Psi}\mathbf{\Phi}^{-1}\mathbf{\Theta}\right]^{-1}\mathbf{f}^1 \\ \mathbf{\Lambda} &= -\left[-\mathbf{\Gamma} + \mathbf{\Psi}\mathbf{\Phi}^{-1}\mathbf{\Theta}\right]^{-1}\mathbf{\Psi}\mathbf{\Phi}^{-1}\mathbf{f}^2 \\ \mathbf{\Xi} &= -\left[-\mathbf{\Phi} + \mathbf{\Theta}\mathbf{\Gamma}^{-1}\mathbf{\Psi}\right]^{-1}\mathbf{\Theta}\mathbf{\Gamma}^{-1}\mathbf{f}^1 \\ \mathbf{\Omega} &= \left[-\mathbf{\Phi} + \mathbf{\Theta}\mathbf{\Gamma}^{-1}\mathbf{\Psi}\right]^{-1}\mathbf{f}^2 \end{aligned} \tag{40}$$

Equation (39) expresses the vectors of eigenstrain and eigenmomentum in each subdivision in terms of the vector of average stress and average velocity. It can be seen that the vectors of the average quantities in equation (39) are composed of $\bar{\alpha}$ times repeated vectors of the averaged quantities. Therefore, equation (39) can be condensed to express the vectors of eigenstrain and eigenmomentum in each subdivision in terms of a 6×1 vector of the average stress and a 3×1 vector of the average velocity. Furthermore, we can also average the vectors of eigenstrain and eigenmomentum over all the subregions to finally get

$$\begin{aligned} \langle\mathbf{E}\rangle_{6\times1} &= \langle\mathbf{\Delta}\rangle_{6\times6}\langle\boldsymbol{\sigma}\rangle_{6\times1} + \langle\mathbf{\Lambda}\rangle_{6\times3}\langle\dot{\mathbf{u}}\rangle_{3\times1} \\ \langle\mathbf{P}\rangle_{3\times1} &= \langle\mathbf{\Xi}\rangle_{3\times6}\langle\boldsymbol{\sigma}\rangle_{6\times1} + \langle\mathbf{\Omega}\rangle_{3\times3}\langle\dot{\mathbf{u}}\rangle_{3\times1} \end{aligned} \tag{41}$$

where

$$\begin{aligned} \langle\mathbf{\Delta}\rangle &= (\mathbf{F}^1)^T\left[-\mathbf{\Gamma} + \mathbf{\Psi}\mathbf{\Phi}^{-1}\mathbf{\Theta}\right]^{-1}\mathbf{F}^1 \\ \langle\mathbf{\Lambda}\rangle &= -(\mathbf{F}^1)^T\left[-\mathbf{\Gamma} + \mathbf{\Psi}\mathbf{\Phi}^{-1}\mathbf{\Theta}\right]^{-1}\mathbf{\Psi}\mathbf{\Phi}^{-1}\mathbf{F}^2 \\ \langle\mathbf{\Xi}\rangle &= -(\mathbf{F}^2)^T\left[-\mathbf{\Phi} + \mathbf{\Theta}\mathbf{\Gamma}^{-1}\mathbf{\Psi}\right]^{-1}\mathbf{\Theta}\mathbf{\Gamma}^{-1}\mathbf{F}^1 \\ \langle\mathbf{\Omega}\rangle &= (\mathbf{F}^2)^T\left[-\mathbf{\Phi} + \mathbf{\Theta}\mathbf{\Gamma}^{-1}\mathbf{\Psi}\right]^{-1}\mathbf{F}^2 \end{aligned} \tag{42}$$

where

$$\left[\mathbf{F}^1\right] = \begin{bmatrix} f^1 & 0 & 0 & 0 & 0 & 0 \\ 0 & f^1 & 0 & 0 & 0 & 0 \\ 0 & 0 & f^1 & 0 & 0 & 0 \\ . & . & . & . & . & . \\ f^2 & 0 & 0 & 0 & 0 & 0 \\ . & . & . & . & . & . \end{bmatrix}$$

$$\left[\mathbf{F}^2\right] = \begin{bmatrix} f^1 & 0 & 0 \\ 0 & f^1 & 0 \\ 0 & 0 & f^1 \\ f^2 & 0 & 0 \\ . & . & . \end{bmatrix}$$

Now we average the consistency conditions over the entire unit cell to express the average strain and average momentum in terms of the average stress and average velocity tensors. Noting that the average of the periodic parts vanishes when taken over the entire unit cell, we have

$$\langle \boldsymbol{\varepsilon} \rangle = \mathbf{D}^0 \langle \boldsymbol{\sigma} \rangle - \langle \mathbf{E} \rangle = \bar{\mathbf{D}} \langle \boldsymbol{\sigma} \rangle + \bar{\mathbf{S}}_1 \langle \dot{\mathbf{u}} \rangle \tag{43}$$

$$\langle \mathbf{p} \rangle = \rho^0 \langle \dot{\mathbf{u}} \rangle - \langle \mathbf{P} \rangle = \bar{\mathbf{S}}_2 \langle \boldsymbol{\sigma} \rangle + \bar{\boldsymbol{\rho}} \langle \dot{\mathbf{u}} \rangle \tag{44}$$

The effective parameters are given by

$$\begin{aligned} \bar{\mathbf{D}} &= \mathbf{D}^0 - \langle \boldsymbol{\Delta} \rangle \\ \bar{\mathbf{S}}_1 &= -\langle \boldsymbol{\Lambda} \rangle \\ \bar{\mathbf{S}}_2 &= -\langle \boldsymbol{\Xi} \rangle \\ \bar{\boldsymbol{\rho}} &= \rho_0 \mathbf{1} - \langle \boldsymbol{\Omega} \rangle \end{aligned} \tag{45}$$

The matrix representation of the effective constitutive relation (43,44) can be transformed into the tensorial representation of the main text (32,33) without any loss of generality.

3.1 Properties of the Constitutive Parameters

Considering equation (38) it can be shown that $\langle \boldsymbol{\Lambda} \rangle$ and $\langle \boldsymbol{\Omega} \rangle$ are hermitian. This implies that $\bar{\mathbf{D}}$ and $\bar{\boldsymbol{\rho}}$ are also hermitian.

Taking a hermitian transpose of equation (45^3):

$$\begin{aligned} \bar{\mathbf{S}}_2^\dagger &= -\langle \boldsymbol{\Xi} \rangle^\dagger \\ &= \left[(\mathbf{F}^2)^T \left[-\boldsymbol{\Phi} + \boldsymbol{\Theta} \boldsymbol{\Gamma}^{-1} \boldsymbol{\Psi} \right]^{-1} \boldsymbol{\Theta} \boldsymbol{\Gamma}^{-1} \mathbf{F}^1 \right]^\dagger \\ &= \left[(\mathbf{F}^2)^T \left[-\boldsymbol{\Gamma} \boldsymbol{\Theta}^{-1} \boldsymbol{\Phi} + \boldsymbol{\Psi} \right]^{-1} \mathbf{F}^1 \right]^\dagger \\ &= (\mathbf{F}^1)^T \left[-\boldsymbol{\Phi} \boldsymbol{\Psi}^{-1} \boldsymbol{\Gamma} + \boldsymbol{\Theta} \right]^{-1} \mathbf{F}^2 \end{aligned}$$

and

$$\begin{aligned} \bar{\mathbf{S}}_1 &= -\langle \boldsymbol{\Lambda} \rangle \\ &= (\mathbf{F}^1)^T \left[-\boldsymbol{\Gamma} + \boldsymbol{\Psi} \boldsymbol{\Phi}^{-1} \boldsymbol{\Theta} \right]^{-1} \boldsymbol{\Psi} \boldsymbol{\Phi}^{-1} \mathbf{F}^2 \\ &= (\mathbf{F}^1)^T \left[-\boldsymbol{\Phi} \boldsymbol{\Psi}^{-1} \boldsymbol{\Gamma} + \boldsymbol{\Theta} \right]^{-1} \mathbf{F}^2 \end{aligned} \tag{46}$$

proving that $\bar{\mathbf{S}}_2^\dagger = \bar{\mathbf{S}}_1$. Since the matrices $[\bar{\mathbf{D}}]$ and $[\bar{\boldsymbol{\rho}}]$ are hermitian, we have $\bar{D}_{ijkl} = \bar{D}^*_{klij}$ and $\bar{\rho}_{ij} = \bar{\rho}^*_{ji}$ where * denotes a complex conjugate. This means that the scalar given by $a = \langle \sigma \rangle_{ij} \bar{D}^*_{ijkl} \langle \sigma \rangle^*_{kl} = \langle \sigma \rangle_{ij} \bar{D}_{klij} \langle \sigma \rangle^*_{kl}$ has a complex conjugate $a^* = \langle \sigma \rangle_{kl} \bar{D}^*_{klij} \langle \sigma \rangle^*_{ij}$. Since the pairs i,j and k,l are symbols upon which summation is carried out, we find that $a = a^*$ or that a is real. Similarly $\langle \dot{u} \rangle_i \bar{\rho}^*_{ij} \langle \dot{u} \rangle^*_j$ can be shown to be a real scalar. The relation $\bar{\mathbf{S}}_2^\dagger = \bar{\mathbf{S}}_1$ implies that $(\bar{S}_2)^*_{ijk} = (\bar{S}_1)_{jki}$.

4. CONCLUSIONS

A method for the homogenization of 3-D periodic elastic composites is presented. The coupled form of the constitutive relation as proposed by Milton and Willis emerges naturally from the present method. We have also shown that the matrices corresponding to the effective compliance and density tensors that are produced by our method are hermitian and that the coupling tensors are hermitian transposes of each other. Moreover, the effective density is shown to be tensorial in nature.

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APPENDIX A. EXPLICIT EXPRESSIONS FOR TENSORS

Equation (16_1) in index notation is

$$\dot{u}_p(\boldsymbol{\xi}) = \Phi_{pj}(\boldsymbol{\zeta})P_j(\boldsymbol{\xi}) + \Theta_{pij}(\boldsymbol{\zeta})E_{ij}(\boldsymbol{\xi}) \tag{47}$$

where $\boldsymbol{\Phi}$ and $\boldsymbol{\Theta}$ for the isotropic reference matrix are given by

$$\Phi_{pj} = \frac{\omega^2}{\rho^0}\left[\frac{c_1^2 - c_2^2}{[\omega^2 - c_1^2\zeta^2]\,[\omega^2 - c_2^2\zeta^2]}\zeta_p\zeta_j + \frac{1}{\omega^2 - c_2^2\zeta^2}\delta_{pj}\right] \tag{48}$$

$$\begin{aligned}\Theta_{pij} \quad &= \quad -\frac{\omega}{2}\left[\left\{\frac{2c_2^2(c_1^2 - c_2^2)}{[\omega^2 - c_2^2\zeta^2][\omega^2 - c_1^2\zeta^2]}\right\}\zeta_i\zeta_j\zeta_p\right. \\ &+ \quad \left.\left\{\frac{c_1^2 - 2c_2^2}{\omega^2 - c_1^2\zeta^2}\right\}\delta_{ij}\zeta_p + \left\{\frac{c_2^2}{\omega^2 - c_2^2\zeta^2}\right\}\{\zeta_i\delta_{jp} + \zeta_j\delta_{ip}\}\right]\end{aligned} \tag{49}$$

In the above expressions $c_1 = \sqrt{(\lambda^0 + 2\mu^0)/\rho^0}$ is the longitudinal wave velocity and $c_1 = \sqrt{\mu^0/\rho^0}$ is the shear wave velocity.

Equation (16_2) in index notation is

$$\sigma_{ij}(\boldsymbol{\xi}) = \Psi_{ijp}(\boldsymbol{\zeta})P_p(\boldsymbol{\xi}) + \Gamma_{ijkl}(\boldsymbol{\zeta})E_{kl}(\boldsymbol{\xi}) \tag{50}$$

where

$$\begin{aligned}\Psi_{ijp} \quad &= \quad -\frac{\omega}{2}\left[\left\{\frac{2c_2^2(c_1^2 - c_2^2)}{[\omega^2 - c_2^2\zeta^2][\omega^2 - c_1^2\zeta^2]}\right\}\zeta_i\zeta_j\zeta_p\right. \\ &+ \quad \left.\left\{\frac{c_1^2 - 2c_2^2}{\omega^2 - c_1^2\zeta^2}\right\}\delta_{ij}\zeta_p + \left\{\frac{c_2^2}{\omega^2 - c_2^2\zeta^2}\right\}\{\zeta_i\delta_{jp} + \zeta_j\delta_{ip}\}\right]\end{aligned} \tag{51}$$

and

$$\Gamma_{ijpq} = C^0_{ijmn}S_{mnkl}C^0_{klpq} \tag{52}$$

where

$$\begin{aligned}S_{mnkl} \quad &= \quad \frac{1}{\rho^0}\left[\frac{1}{4(\omega^2 - c_2^2\zeta^2)}\{\zeta_m\delta_{nk}\zeta_l + \zeta_m\delta_{nl}\zeta_k + \zeta_n\delta_{mk}\zeta_l + \zeta_n\delta_{ml}\zeta_k\}\right. \\ &+ \quad \frac{-(c_1^2 - 2c_2^2)}{2c_2^2(3c_1^2 - 4c_2^2)}\delta_{mn}\delta_{kl} + \frac{c_1^2 - c_2^2}{[\omega^2 - c_2^2\zeta^2][\omega^2 - c_1^2\zeta^2]}\zeta_m\zeta_n\zeta_k\zeta_l \\ &+ \quad \left.\frac{1}{4c_2^2}\{\delta_{mk}\delta_{nl} + \delta_{ml}\delta_{nk}\}\right]\end{aligned}$$

It can be seen from the symmetries of the $\mathbf{S}$ tensor that the above tensors satisfy the following properties

$$\Theta_{pmn} = \Psi_{mnp}; \quad \Gamma_{mnkl} = \Gamma_{nmkl} = \Gamma_{mnlk} = \Gamma_{klmn} \tag{53}$$