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A generalized theory of elastodynamic homogenization for periodic media

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Abstract

For periodically inhomogeneous media, a generalized theory of elastodynamic homogenization is proposed so that even the long-wavelength and low-frequency asymptotic expansions of the resulting effective (or macroscopic) motion equation can, approximately but simultaneously, capture all the acoustic and some of the optical branches of the microscopic dispersion curve. The key to constructing the generalized theory resides in incorporating new kinematical degrees of freedom in conjunction with rapidly oscillating body forces as microscopic and macroscopic loadings while satisfying an energetical consistency constraint reminiscent of Hill-Mandel lemma. By this constraint, an effective displacement field is naturally defined as the projection of a microscopic one onto the dual to the space of body forces. To illustrate these results, a two-phase string is studied in detail.

Keywords: homogenization, Willis theory, generalized continua, optical branches, band gaps

1. Introduction

The elastodynamic homogenization approaches reported up to now in the literature are observed to run into difficulties when being used to model dynamical effects over a wide frequency range.

1. The classical lowest-order Long-Wavelength (LW) Low-Frequency (LF) homogenization approaches (Bensoussan et al., 1978; Sanchez-Palencia, 1980) yield a homogeneous substitution Cauchy medium which misses all dispersive effects and all internal resonances, i.e., all optical oscillation modes.

2. The higher-order LW-LF asymptotic homogenization approaches (Boutin and Auriault, 1993; Andrianov et al., 2008) lead to effective strain-gradient media which can model well dispersive behaviors and size effects but are valid only near the acoustic branches independently of the order of the asymptotic approximations used.

3. The high-frequency asymptotic approaches (Daya et al., 2002; Craster et al., 2010; Nolde et al., 2011; Antonakakis et al., 2014; Colquitt et al., 2014; Boutin et al., 2014) are successful in capturing high-frequency optical modes but still valid only in the vicinity of some finite frequency.

4. The high-contrast asymptotic approaches (Auriault and Bonnet, 1985; Smyshlyaev, 2009; Auriault and Boutin, 2012) have a wide frequency validity domain englobing an infinite number of optical branches. However, the corresponding effective behavior is complex and nonlocal in time.

5. The non-asymptotic theory of Willis (1997, 2011) yields exactly the whole dispersion curve. Nonetheless, the described effective fields are
only relevant for low frequencies (Srivastava and Nemat-Nasser, 2014; Nassar et al., 2015b).

The main purpose of the present paper is to construct a generalized theory of elastodynamic homogenization for periodic media which improves the quality of the Willis effective behavior as an approximation to the microscopic behavior in a way that LW-LF asymptotic expansions become able to capture, approximately but simultaneously, all the acoustic and some of the optical branches of the microscopic dispersion curve. To achieve this purpose, new kinematical Degrees Of Freedom (DOFs) are taken into account so as to describe some short-wavelength components of the microscopic displacement field which become dominant at high frequencies. The new DOFs are excited by incorporating various rapidly oscillating body forces on the microscale and on the macroscale under an energetical consistency constraint hereafter called Energy Equivalency Principle (EEP). The EEP is a balance between the microscopic and macroscopic virtual works and is later proven to yield a generalized version of the well-known Hill-Mandel lemma. With respect to Willis theory, we underline two major differences. First, the incorporated loadings are much richer than those employed by Willis (1997, 2011). This has the consequence of reducing the error committed during the upscaling process and providing an extended frequency validity domain. Second, the EEP concerns virtual works and not their expectancies. From the physical standpoint, this leads to a clear distinction between the macroscale and the microscale in terms of wavelengths. Nevertheless, it should be pointed out that the generalized theory presented here is by construction limited to periodically inhomogeneous media while Willis theory is formally valid both
for periodically and randomly inhomogeneous media.

The paper is organized as follows. In section 2, we recall some geometrical elements useful for describing periodic media, summarize the equations governing the kinematics and dynamics of them, and simplify these equations by using Bloch-wave expansions. The main body of the generalized theory is presented in section 3. The EEP is first postulated; the space of admissible body forces is then defined as the set of macroscopically applied loadings; the effective displacement field associated to a microscopic displacement is obtained by the EEP and proven to be an improvement over the one defined by Willis; the effective motion equation is finally derived in a formal way and a Hill-Mandel relation is demonstrated. In section 4, an analytical LW-LF asymptotic approximation to the effective motion equation is given for a particular 1D two-phase string. Exact and approximate dispersion curves are plotted and compared. It appears then how the resulting asymptotic model, though based on LF expansions, can simultaneously capture acoustic and optical branches while conserving a low-order local motion equation.

2. Preliminaries

In this section, some geometrical elements useful for the study of periodic media are recalled. The governing equations of linear elasticity are recapitulated. Bloch-wave expansions of fields and work are also introduced.

2.1. Geometry and periodicity

Let $\Omega$ be a $d$-dimensional infinite body. Define $\mathcal{E}$ as the vector space of translations acting on the points of $\Omega$. Given $d$ independent translations $(b_j)_{j=1,\ldots,d}$, denote by $\mathcal{R}$ the subset of $\mathcal{E}$ obtained by integer combinations of
these vectors. The subset $\mathcal{R}$ is called a lattice. Then, a scalar, vector or tensor field $h$ defined over $\Omega$ is said to be $\mathcal{R}$-periodic if and only if it satisfies $h(x + r) = h(x)$ for all points $x \in \Omega$ and all translations $r \in \mathcal{R}$. Accordingly, $h$ needs being defined only over a unit cell

$$T = \left\{ x_o + r \bigg| r = \sum_{j=1}^{d} r_j b_j, -1/2 \leq r_j < 1/2 \right\} \subset \Omega,$$

where $x_o$, its center, is an arbitrary point of $\Omega$. Note that while $\mathcal{R}$-periodicity is well defined, the choice of $b_j$ and $T$ is not unique.

Symbolize by $\mathcal{E}^*$ the dual space of $\mathcal{E}$. A wavenumber $k \in \mathcal{E}^*$ acting on a translation $r \in \mathcal{E}$ produces a phase shift $k \cdot r$ where $(\cdot)$ is the usual dot product. Now, points of $\Omega$ and vectors of $\mathcal{E}$ can be identified after choosing some origin $x_o$. In what follows, we drop $x_o$ so as to write $k \cdot x$ instead of $k \cdot (x - x_o)$ for simplicity. The reciprocal lattice $\mathcal{R}^*$ of the direct lattice $\mathcal{R}$ is defined as the subset of $\mathcal{E}^*$ consisting of wavenumbers $\xi$ such that $e^{i\xi \cdot x}$ is $\mathcal{R}$-periodic, with $i^2 = -1$. Also of interest is the first Brillouin zone $T^*$ defined as the set of wavenumbers closer to the null wavenumber than to any other wavenumber of $\mathcal{R}^*$, i.e.,

$$T^* = \{ k \in \mathcal{E}^* ||k|| < ||k - \xi||, \forall \xi \in \mathcal{R}^* - \{0\} \}.$$

This zone is uniquely defined and independent of $T$.

A function $h$ defined over $\Omega$ can be expanded into plane waves over $\mathcal{E}^*$ such that

$$h(x) = \int_{\mathcal{E}^*} \tilde{h}_k e^{ik \cdot x} \, dk.$$

In particular, when $h$ is $\mathcal{R}$-periodic, it can be written as the Fourier series

$$h(x) = \sum_{\xi \in \mathcal{R}^*} \tilde{h}_\xi e^{i\xi \cdot x}.$$
Having this in mind, with respect to $R$, $T^*$ can be seen as the support of slowly varying fields. In particular, among $R$-periodic functions, only constants have their wavenumber contained in $T^*$, i.e., $T^* \cap R^* = \{0\}$.

Finally, call a Bloch wave, of wavenumber $k$ and amplitude $\tilde{h}_k(x)$, a function $h_k(x)$ of the form

$$h_k(x) = \tilde{h}_k(x)e^{ik \cdot x},$$

where $\tilde{h}_k(x)$ is $R$-periodic.

2.2. Constitutive and motion equations

Letting $u(x, t)$ be the displacement vector for a point $x \in \Omega$ at instant $t$, the strain field $\epsilon$ and velocity field $v$ are derived according to

$$\epsilon = \nabla \otimes s u, \quad v = \dot{u},$$

where $\nabla$ is the space gradient operator, $\otimes$ denotes the tensor product, the superscripted “$s$” indicates symmetrization and a superscripted dot symbolizes differentiation with respect to time. The stress tensor $\sigma$ and momentum density $p$ are then given by the local constitutive equations of $\Omega$:

$$\sigma = C : \epsilon, \quad p = \rho v,$$

with $C$ and $\rho$ being the elastic stiffness tensor and the scalar mass density, respectively, and the colon ($: \sigma$) standing for double contraction.

The motion equation of $\Omega$ reads

$$\nabla \cdot \sigma + f = \dot{p},$$

where $(\nabla \cdot)$ is the divergence operator and $f$ is a field of externally applied body forces. We shall mostly work with harmonic fields of frequency $\omega$. 
Therefore, all time derivatives can be substituted by $i\omega$-multiplications and time dependency can be dropped henceforth. The motion equation of $\Omega$ becomes the Helmholtz equation

$$\nabla \cdot [C(x) : (\nabla \otimes^s u(x))] + f(x) = -\omega^2 \rho(x) u(x)$$ (2.1)

where we have displayed $x$-dependencies and omitted $\omega$-dependencies.

In this work, the homogenization of $\Omega$ amounts to finding the motion equation, hereafter called “effective motion equation”, of a homogeneous medium substituting the initial inhomogeneous one, under an energy equivalency constraint to be specified.

2.3. Bloch-wave expansions

The superposition principle makes it possible to work with elementary, such as plane-wave, body forces instead of arbitrary ones $f(x)$. It is however more convenient, for reasons that will become clear, to work with Bloch-wave body forces. Then, let $f_k(x)$ be an element of the Bloch-wave expansion of $f(x)$ such that

$$f(x) = \int_{T^*} f_k(x) \, d^d k \equiv \int_{T^*} \tilde{f}_k(x) e^{i k \cdot x} \, d^d k,$$ (2.2)

where $\tilde{f}_k(x)$ is $\mathcal{R}$-periodic and the symbol $\equiv$ stands for equality by definition.

For a given $k \in T^*$, the motion equation for a Bloch-wave body force takes the form

$$\nabla \cdot [C(x) : (\nabla \otimes^s u_k(x))] + \tilde{f}_k(x) e^{i k \cdot x} = -\omega^2 \rho(x) u_k(x).$$

We now assume that $C$ and $\rho$ are $\mathcal{R}$-periodic so that the solution $u_k(x)$ can be written as

$$u_k(x) = \tilde{u}_k(x) e^{i k \cdot x}$$
with an $\mathbb{R}$-periodic amplitude $\tilde{u}_k(x)$ (Gazalet et al., 2013). In other words, to the expansion (2.2), there corresponds a similar Bloch-wave expansion of the solution to (2.1):

$$u(x) = \int_{T^*} u_k(x) \, d^d k = \int_{T^*} \tilde{u}_k(x)e^{i k \cdot x} \, d^d k,$$

(2.3)

with $u_k(x)$ being the displacement field over $\Omega$ subjected to $f_k(x)$. In contrast, except for a homogeneous body, there are no similar results for plane waves.

Given the Bloch-wave form of $u_k$, and simplifying the phase factor $e^{i k \cdot x}$, the motion equation becomes, in terms of $\tilde{u}_k(x)$ and $\tilde{f}_k(x)$,

$$(\nabla + i k) \cdot \{C(x) : [(\nabla + i k) \otimes^* \tilde{u}_k(x)]\} + \tilde{f}_k(x) = -\omega^2 \rho(x) \tilde{u}_k(x).$$

(2.4)

Last, the $x$-dependencies of Bloch amplitudes for displacements and body forces were explicitly annotated. In what follows, all fields are understood to be $x$-dependent unless otherwise stated.

2.4. External work

Define the virtual work of external body forces $f$ associated with a virtual displacement field $u$ by

$$\int_{\Omega} f \cdot u^*$$

where a superscripted * denotes complex conjugation. Also, introduce the averaging operator $\langle \rangle$ by

$$\langle h \rangle = \frac{1}{|T|} \int_T h(x) \, d^d x$$

for all $\mathbb{R}$-periodic functions $h$. Note that $\langle \rangle$ is independent of the choice of $T$ and is ill-defined for non-$\mathbb{R}$-periodic functions. Plancherel’s identity for
Fourier transform and Parseval’s identity for Fourier series deliver then a similar identity for Bloch-wave expansions:

\[
\int_{\Omega} \mathbf{f} \cdot \mathbf{u}^* = (2\pi)^d \int_{T^*} \left\langle \tilde{f}_k \cdot \tilde{u}_k^* \right\rangle \, d^d k = \frac{(2\pi)^d}{|T|} \int_{T^*} \int_T \tilde{f}_k(x) \cdot \tilde{u}_k^*(x) \, d^dx \, d^dk.
\]

Consequently, in defining the energetically equivalent effective behavior, we can work with fields of a single Bloch wavenumber \( k \in T^* \) and then apply the superposition principle even though work is quadratic and not linear.

3. A general theory

In this section, the energy equivalency principle (EEP), the corner stone of the present approach, is first postulated, given a simple form and exploited to define the effective displacement field. A formal derivation of the effective motion equation is then presented. The effective constitutive behavior is nonlocal in both space and time which raises questions about its uniqueness (Fietz and Shvets, 2010; Willis, 2011). In order to avoid this difficulty, we will be interested only in the effective motion equation which is unique. Nonetheless, we will derive expressions for the generalized stress, momentum, velocity and strain measures which are, in particular, needed for determining an effective constitutive law.

3.1. Energy equivalency

In classical static or quasi-static homogenization, an energy equivalency relation, known as Hill-Mandel lemma, is proven for a family of boundary conditions prescribed on a representative volume element as macroscopic loadings. Once the boundary conditions have been specified, Hill-Mandel
lemma can be used to define, by duality, the macroscopic stress in a strain-based approach or the macroscopic strain in a stress-based approach. In the present formulation, admissible body forces applied globally to $\Omega$ instead of boundary conditions are taken to be macroscopic loading. Then, an EEP is postulated so as to dualize body forces and displacements. This duality will allow us to define the macroscopic displacement field, called $\mathbf{D}$, in terms of the microscopic one $\mathbf{u}$, once admissible body forces have been imposed.

Let $\mathcal{F}$ be the space of Bloch amplitudes $\tilde{f}_k$, involved in (2.2), of admissible body forces. The elements of $\mathcal{F}$ are seen as external loadings likely to be applied to $\Omega$. Note that they will remain the same after the scale transition. The space $\mathcal{F}$ acts as a parameter of the approach to be elaborated and needs to be chosen adequately. Next, let $\mathcal{F}^*$, the space dual to $\mathcal{F}$, be the space of Bloch amplitudes $\tilde{D}_k$ of admissible effective displacement fields. For a given microscopic displacement field $\mathbf{u}$, the corresponding effective (or macroscopic) displacement field is defined as the unique admissible displacement such that

$$\int_{\Omega} \mathbf{f} \cdot \mathbf{D}^* = \int_{\Omega} \mathbf{f} \cdot \mathbf{u}^*$$

(3.1)

for all admissible virtual body forces $\mathbf{f}$ (i.e., $\tilde{f}_k \in \mathcal{F}$, for all $k \in T^*$).

Physically, the EEP (3.1) can be interpreted as requiring that the effective displacement field $\mathbf{D}$ associated to a given microscopic field $\mathbf{u}$ be such that the work done by every admissible virtual body force $\mathbf{f}$ in the course of $\mathbf{D}$ is equal to the one done by $\mathbf{f}$ in the course of $\mathbf{u}$. Geometrically, the EEP (3.1) simply means that $\mathbf{D}$ is the projection of $\mathbf{u}$ onto the space of admissible displacements (figure 1). On the basis of the EEP (3.1), a generalized Hill-Mandel lemma will be proven in subsection 3.4.

Using the Bloch decomposition (2.5), the EEP (3.1) can be equivalently
written in terms of Bloch amplitudes as

$$
\forall k \in T^*, \quad \forall \tilde{f}_k \in \mathcal{F}, \quad \langle \tilde{f}_k \cdot \tilde{D}_k \rangle = \langle \tilde{f}_k \cdot \tilde{u}_k \rangle.
$$

(3.2)

Figure 1: The effective displacement field $D$ associated to a given microscopic one $u$ is geometrically interpreted as the projection of the latter onto the space of admissible displacements. Spaces $\mathcal{F}$ and $\mathcal{F}^*$ are isomorphic and, here, are taken to be equal up to a change in units.

3.2. Effective displacement field

Bearing in mind the EEP (3.1), choosing the space $\mathcal{F}$ of admissible body forces becomes a key step toward elaborating a generalized theory. The choice of $\mathcal{F}$ depends ultimately on the degree of accuracy with which $D$ is required to approximate $u$. The bigger $\mathcal{F}$ is, the closer $D$ is to $u$. When all body forces are considered as admissible, the relation (3.1) implies $D = u$ and the
effective medium is trivially the original one. In what follows, we study the rather general case of practical importance where $\mathcal{F}$ is finite-dimensional and show how $D$ derives from (3.1) correspondingly.

3.2.1. Admissible body forces

Given $N$ linearly independent, $k$- and $\omega$-independent, $\mathcal{R}$-periodic vector fields $\phi_i$ with $i = 1 \ldots N$, a Bloch-wave body force field $f_k$ is admissible if and only if it has an $\mathcal{R}$-periodic Bloch amplitude $\tilde{f}_k$ of the form

$$\tilde{f}_k(x) = \sum_{i=1}^{N} \tilde{f}_i^k \phi_i(x),$$

(3.3)

where the $\tilde{f}_i^k$ are constants. The space $\mathcal{F}$ is therefore of dimension $N$.

With no loss of generality, let the subset $(\phi_i)_{i=1 \ldots d}$, where $d$ is the dimension of $\Omega$, be formed of constant vectors and constitute a basis for $\mathcal{E}$. We call $\tilde{F}_k$ the constant component of $\tilde{f}_k$ and write

$$\tilde{f}_k(x) = \sum_{i=1}^{d} \tilde{f}_i^k \phi_i(x) + \sum_{i=d+1}^{N} \tilde{f}_i^k \phi_i(x) \equiv \tilde{F}_k + \tilde{f}_k^\alpha \phi_\alpha(x).$$

(3.4)

Above and from now on, the repeated Greek indices are understood to be summed over from $d+1$ to $N$ whereas the Latin ones run from 1 to $N$ unless otherwise specified. Integrating with respect to $k$ over $T^*$, we obtain the generic form of admissible body forces:

$$f(x) = F(x) + f^\alpha(x) \phi_\alpha(x).$$

Of most importance is the fact that fields $F$ and $f^\alpha$ have their supports contained in $T^*$. As such, they have wavelengths at least twice as large as the characteristic length of a unit cell. Consequently, the DOFs $F$ and $f^\alpha$ of admissible body forces are said to be “macroscopic”. These DOFs are carried
by $\mathcal{R}$-periodic shape functions, the $\phi_\alpha$, describing the ways in which $f$ can vary on the microscale. For example, taking $N = d$, we have $f(x) = F(x)$ implying that body forces are not allowed to vary on the microscale. As another example, setting $N = d + 1$ and $\phi_{d+1}(x) = \rho(x)e$, where $e$ is a vertically oriented vector, we have $f(x) = F(x) + f^{d+1}(x)\rho(x)e$ so that the admissible variations of body forces on the microscale are gravitational.

### 3.2.2. Effective displacement field by the EEP

From now on, we assume that the $\phi_\alpha$ form an orthonormal basis of $\mathcal{F}$ so that
\[
\forall i, j \in \{1, \ldots, N\}, \quad \langle \phi_i \cdot \phi_j^* \rangle = \delta_{ij},
\]
where $\delta_{ij}$ is the Kronecker delta. For $\beta \in \{1, \ldots, d\}$, $\phi_\beta$ being constant entails
\[
\forall \alpha \in \{d+1, \ldots, N\}, \quad \langle \phi_\alpha \rangle = 0,
\]
meaning that being orthogonal to a constant is equivalent to having a zero average.

Injecting (3.4) in the expression of the virtual work, we obtain
\[
\begin{align*}
\langle \hat{f}_k \cdot \hat{u}_k^* \rangle &= \langle \hat{F}_k \cdot \hat{u}_k^* \rangle + \langle \hat{f}_k^\alpha \phi_\alpha \cdot \hat{u}_k^* \rangle \quad \text{(by orthogonality)} \\
&= \hat{F}_k \cdot \langle \hat{u}_k \rangle^* + \hat{f}_k^\alpha \langle \phi_\alpha^* \cdot \hat{u}_k \rangle^* \quad \text{(by constancy)} \\
&= \hat{F}_k \cdot \hat{U}_k^* + \hat{f}_k^\alpha \hat{u}_k^{\alpha^*} \quad \text{(by definition (3.5))} \\
&= \langle \hat{F}_k \cdot \hat{U}_k^* \rangle + \langle \hat{f}_k^\alpha \phi_\alpha \cdot (\hat{u}_k^\beta \phi_\beta)^* \rangle \quad \text{(by orthogonality)} \\
&= \langle \hat{f}_k \cdot (\hat{U}_k + \hat{u}_k^\beta \phi_\beta)^* \rangle, \quad \text{(by orthogonality)}
\end{align*}
\]
with
\[
\hat{U}_k \equiv \langle \hat{u}_k \rangle, \quad \hat{u}_k^\beta \equiv \langle \phi_\beta^* \cdot \hat{u}_k \rangle.
\]
Then, it follows from (3.2) that

\[ \tilde{D}_k(x) = \tilde{U}_k + \tilde{u}_k^\beta \phi_\beta(x). \]

Finally, summing over \( T^* \), it comes that

\[ D(x) = U(x) + u^\beta(x) \phi_\beta(x). \]

The above expression of the effective displacement field results from the EEP combined with a particular choice of admissible body forces. It contains the classical translational displacement vector \( U \) and additional generalized “displacements” \( u^\beta \) carried by the shape functions \( \phi_\beta \). Once more, the shape functions define the way in which \( D \) varies on the microscale whereas the slowly varying DOFs \( U \) and \( u^\beta \) describe how \( D \) varies on the macroscale.

Willis (2011) proposed a homogenization theory in which shape functions are taken to be \( \phi_i(x) = w(x)e_i \), for \( i \in \{1,...d\} \), where \( w(x) \) is a fixed \( \mathcal{R} \)-periodic function and the \( e_i \) form a basis for \( \mathcal{S} \). Taking \( w \equiv 1 \) yields the unweighted theory of 1997 (Willis, 1997) and amounts to taking \( f = F \) and \( D = U \). Here, we combine both the weighted and unweighted Willis theories and use even more general shape functions. As a consequence, \( D \) is a better approximation of \( u \) than \( U \) as will be seen in more detail.

3.2.3. Effective displacement field through error minimization

First of all, rewriting (3.2) in the equivalent form

\[ \forall \tilde{f}_k \in \mathcal{F}, \quad \langle \tilde{f}_k \cdot (\tilde{u}_k - \tilde{D}_k)^* \rangle = 0, \]

it is clear that \( \tilde{u}_k - \tilde{D}_k \) is orthogonal to \( \mathcal{F} \) and \( \tilde{D}_k \) acts as the orthogonal projection of \( \tilde{u}_k \) onto \( \mathcal{F}^* \) (figure 1). Using the Pythagorean theorem, it is
easy to see that for any $\mathcal{R}$-periodic field $h \in \mathcal{F}^*$,

$$
\langle (\tilde{u}_k - h) \cdot (\tilde{u}_k - h)^* \rangle = \langle (\tilde{u}_k - \tilde{D}_k) \cdot (\tilde{u}_k - \tilde{D}_k)^* \rangle + \langle (\tilde{D}_k - h) \cdot (\tilde{D}_k - h)^* \rangle
\geq \langle (\tilde{u}_k - \tilde{D}_k) \cdot (\tilde{u}_k - \tilde{D}_k)^* \rangle.
$$

Thus,

$$
\tilde{D}_k = \arg \min_{h \in \mathcal{F}^*} \langle (\tilde{u}_k - h) \cdot (\tilde{u}_k - h)^* \rangle. \quad (3.6)
$$

This shows that the effective displacement Bloch amplitude is the best admissible approximation to the microscopic one. Consequently, the effective displacement field $D$, associated to a microscopic displacement field $u$, can be seen as the best admissible approximation to $u$. Note that this global optimal argument definition (where the support is $\Omega$) is different from the local one introduced elsewhere (Forest and Sab, 1998; Forest, 2006) (where the support is a representative volume element) despite an apparent resemblance.

The preceding definition of the effective displacement field concretizes the intuition that the richer the DOFs of the generalized substitution medium are, the closer $D$ is to $u$:

if $\mathcal{F}_1 \subset \mathcal{F}_2$ then $\min_{h \in \mathcal{F}^*_2} \langle (\tilde{u}_k - h) \cdot (\tilde{u}_k - h)^* \rangle \leq \min_{h \in \mathcal{F}_1} \langle (\tilde{u}_k - h) \cdot (\tilde{u}_k - h)^* \rangle$.

In this sense, the generalized substitution medium to be obtained by our theory is more realistic than the Willis substitution medium in the above minimal error sense, at the cost of an additional kinematical complexity (see figure 2).

A remark is now in order. We have used a scalar product on the space of body forces twice up till now: once to identify $\mathcal{F}$ and $\mathcal{F}^*$ and once to orthonormalize the set of shape functions. This scalar product is not unique and can be modified by adding a weighting function such as mass density
Figure 2: Plots of the real parts of the microscopic ($\tilde{u}$), Willis ($\tilde{U}$), and generalized ($\tilde{D}$) Bloch displacement amplitudes over one period for 3 eigenmodes: $(k = 0, \omega = \omega_1(0))$ (top), $(k = \pi/2a, \omega = \omega_2(\pi/2a))$ (middle), $(k = 0, \omega = \omega_2(0))$ (bottom). Two shape functions have been used: a constant and a sine wave. Details are given in section 4.

for instance. Note that such choice has influence neither on the definition of the DOFs $u^\alpha$, nor on the effective motion equation to be found. It simply changes the above quadratic error function and determines the mapping $(u^i)_{i=1...N} \mapsto D$. 
3.2.4. Effective displacement field under infinite scale separation

It is of interest to examine what $D$ becomes under the hypothesis of infinite scale separation, namely, when $k \to 0$ and $\omega \to 0$. It is known that in this case, to the lowest order, the displacement field depends only on the “slow variable” (refer to Boutin and Auriault, 1993, for instance). In terms of Bloch amplitudes, this means that $\tilde{u}_k$ is constant. Consequently,

$$\bar{U}_k = \langle \tilde{u}_k \rangle = \tilde{u}_k,$$

$$\tilde{u}_\alpha^k = \langle \phi^*_\alpha \cdot \tilde{u}_k \rangle = \langle \phi^*_\alpha \rangle \cdot \tilde{u}_k = 0.$$ 

Therefore, the translational DOF $U$ is the only non-null component of $D$, to the lowest order. The use of a generalized kinematics is hence justified only under weak scale separation or for high frequencies when microscopic deformation modes become significant. Otherwise, it is enough to keep track of $U$ exclusively as in the unweighted Willis theory. As a matter of fact, it has been observed that a periodic medium was “homogenizable” in the Willis sense over the acoustic and the first optical branches only (Srivastava and Nemat-Nasser, 2014; Nassar et al., 2015b). For higher frequencies, one needs to use non-uniform shape functions.

3.3. Effective motion equation

Having specified body forces, the motion equation (2.4) becomes

$$(\nabla + ik) \cdot \{ C(x) : (\nabla + ik) \otimes \tilde{u}_k(x) \} + \tilde{F}_k + f^\alpha_k(x) \phi_\alpha(x) = -\omega^2 \rho(x) \tilde{u}_k(x),$$

which needs to be solved over $\Omega$. Since $\tilde{u}_k$ is $\mathcal{B}$-periodic, it is enough to solve the above equation over a unit cell $T$ under periodic boundary conditions.
Let $g_k$ be the corresponding periodic second order Green operator. Then,

$$ \tilde{u}_k(y) = \frac{1}{T} \int_T g_k(y, x) \cdot \tilde{f}_k(x) \, d^d x $$

$$ = \left( \frac{1}{T} \int_T g_k(y, x) \, d^d x \right) \cdot \tilde{F}_k + \left( \frac{1}{T} \int_T g_k(y, x) \cdot \phi_\alpha \, d^d x \right) \tilde{f}_k^\alpha $$  (3.7)

which, combined with (3.5), delivers the following expressions for the components of the macroscopic displacement field:

$$ \tilde{U}_k = \left( \langle \langle g_k(y, x) \rangle \rangle \right) \cdot \tilde{F}_k + \left( \langle \langle g_k(y, x) \cdot \phi_\alpha(x) \rangle \rangle \right) \tilde{f}_k^\alpha, $$

$$ \tilde{u}_k^\beta = \left( \langle \langle \phi^*_\beta(y) \cdot g_k(y, x) \rangle \rangle \right) \cdot \tilde{F}_k + \left( \langle \langle \phi^*_\beta(y) \cdot g_k(y, x) \cdot \phi_\alpha(x) \rangle \rangle \right) \tilde{f}_k^\alpha, $$  (3.8)

where $\langle \langle \rangle \rangle$ means averaging with respect to both $x$ and $y$.

The Green operator of the effective medium $G_k$ is given by the last two equalities which can be written concisely as

$$ \tilde{u}_k^i = G_{ij}^k \tilde{f}_k^j, $$

where no distinction is made between the classical and generalized DOFs (recall that $\tilde{U}_k = \sum_{j=1}^d \tilde{u}_k^j \phi_j$). Inverting the preceding equation delivers the effective motion equation in Fourier domain:

$$ Z_{ij}^k \tilde{u}_k^j = \tilde{f}_k^i, $$  (3.9)

where $Z_k$, the inverse of $G_k$, is called the effective impedance. It depends implicitly on the frequency $\omega$. By summing over $k \in T^*$ and over $\omega$, we obtain the effective motion equation in $x$ and $t$ as

$$ Z^{ij}(x, t) * u^j(x, t) = f^i(x, t), $$

where $Z(x, t)$ is an integro-differential operator and $*$ denotes convolution product with respect to space and time. The effective motion equation is
hence nonlocal in both space and time and involves long wavelengths ($k \in T^*$) only. This generalizes equation (3.28) derived by Willis (1997) for periodic media.

3.4. Internal work

As mentioned earlier, it is not essential for achieving the main purpose of the present work to derive an explicit expression for the underlying effective constitutive law which is not unique as in the theory of Willis. However, it is of interest to specify the macroscopic stress, momentum, strain and velocity measures that an effective constitutive law involves. In addition, these generalized macroscopic measures will be shown to be related to their microscopic counterparts through an extended Hill-Mandel relation.

3.4.1. Generalized stress and momentum measures

Said measures are taken to be the ones involved in the effective motion equation written as a conservation law equivalent to (3.9). Starting with the microscopic motion equation

$$\left( \nabla + ik \right) \cdot \tilde{\sigma}_k + \tilde{F}_k + \tilde{f}_k^\alpha \phi_\alpha = i\omega \tilde{p}_k, \quad (3.10)$$

where $\tilde{\sigma}_k$ and $\tilde{p}_k$ are the Bloch amplitudes of stress and momentum, we take its volume average over a unit cell to obtain, with the help of the divergence theorem,

$$ik \cdot \tilde{\Sigma}_k + \tilde{F}_k = i\omega \tilde{P}_k. \quad (3.11)$$

This is the first effective motion equation involving the classical macroscopic stress and momentum measures:

$$\tilde{\Sigma}_k \equiv \langle \sigma_k \rangle, \quad \tilde{P}_k \equiv \langle \tilde{p}_k \rangle.$$
Further, projecting equation (3.10) onto the space spanned by the other shape functions $\phi^\beta$ gives rise to

$$i k \cdot \left\langle \phi^{\beta^*} \cdot \tilde{\sigma}_k \right\rangle - \left\langle \left( \nabla \otimes^s \phi^{\beta^*} \right) : \tilde{\sigma}_k \right\rangle + \tilde{f}^\beta_k = i \omega \left\langle \phi^{\beta^*} \cdot \tilde{p}_k \right\rangle,$$

where, for simplicity, we have assumed the continuity of $\phi^\beta$ so that the boundary term vanishes. The generalized stress and momentum measures can be identified as

$$\tilde{\sigma}_k^\beta \equiv \left\langle \phi^{\beta^*} \cdot \tilde{\sigma}_k \right\rangle, \quad \tilde{s}_k^\beta \equiv - \left\langle \left( \nabla \otimes^s \phi^{\beta^*} \right) : \tilde{\sigma}_k \right\rangle, \quad \tilde{p}_k^\beta \equiv \left\langle \phi^{\beta^*} \cdot \tilde{p}_k \right\rangle.$$

The additional motion equation becomes then simply

$$\tilde{s}_k^\beta + i k \cdot \tilde{\sigma}_k^\beta + \tilde{f}_k^\beta = i \omega \tilde{p}_k^\beta.$$

(3.12)

Note that equations (3.11) and (3.12) on one hand, and (3.9) on the other, are related to one another through a non-unique effective constitutive law whose characterization is beyond the purpose of the present work (see the discussion by Willis, 2011, 2012).

In summary, the motion equations in the space domain are given by

$$\nabla \cdot \Sigma + F = i \omega P,$$

(3.13)

$$s^\beta + \nabla \cdot \sigma^\beta + f^\beta = i \omega p^\beta.$$

These equations are a micromechanical version of the “equations of equilibrium” phenomenologically derived by Germain (1973).

### 3.4.2. Generalized strain and velocity measures

Said measures are obtained by duality. The virtual work theorem combined with the EEP yields

$$\left\langle \sigma_k : \varepsilon_k^\beta - \tilde{p}_k \cdot \tilde{v}_k^\beta \right\rangle = \left\langle \tilde{f}_k \cdot \tilde{u}_k^\beta \right\rangle = \tilde{F}_k \cdot \tilde{U}_k^\beta + \tilde{f}_k^\alpha \tilde{u}_k^\alpha^*.$$

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where $\tilde{\varepsilon}_k$ and $\tilde{v}_k$ are the Bloch amplitudes of the strain and velocity fields, respectively, given by

$$
\tilde{\varepsilon}_k = (\nabla + ik) \otimes^s \tilde{u}_k, \quad \tilde{v}_k = i\omega \tilde{u}_k.
$$

Substituting body forces by the corresponding stress and momentum measures according to (3.12) delivers

$$
\langle \tilde{\sigma}_k : \tilde{\varepsilon}_k^* - \tilde{p}_k \cdot \tilde{v}_k^* \rangle = \tilde{\Sigma}_k : (ik \otimes^s \tilde{U}_k)^* - \tilde{P}_k \cdot (i\omega \tilde{U}_k)^*
$$

$$
+ \tilde{\sigma}_k^\alpha \cdot (ik \tilde{u}_k^\alpha)^* - \tilde{p}_k^\alpha (i\omega \tilde{u}_k^\alpha)^* - \tilde{s}_k^\alpha \tilde{u}_k^{\alpha*}.
$$

Summing over $k$, and using Placherel’s identity, we obtain a generalized version of the Hill-Mandel lemma:

$$
\int_\Omega \{ \sigma : \varepsilon^* - p \cdot v^* \}
$$

$$
= \int_\Omega \{ \Sigma : (\nabla \otimes^s U)^* - P \cdot (i\omega U)^* + \sigma^\alpha \cdot (\nabla \tilde{u}^\alpha)^* - p^\alpha (i\omega u^\alpha)^* - s^\alpha u^{\alpha*} \}.
$$

(3.14)

This result is valid for all virtual couples $(\sigma, p)$ equilibrated by an admissible body force field and for all couples $(\varepsilon, v)$ derived from an arbitrary displacement field $u$. From the above relation, we identify the classical macroscopic measures of strain and velocity as $\nabla \otimes^s U$ and $i\omega U$ while the generalized ones are $\nabla \tilde{u}^\alpha$, $u^\alpha$ and $i\omega u^\alpha$.

Finally, the constructed macroscopic fields meet the most fundamental requirements for them to be interpreted as stresses, momenta, strains and velocities since they rigorously satisfy local balance and compatibility equations. Nonetheless, how to physically interpret and measure these quantities in a precise way ultimately depends on the chosen set of shape functions. More details are given in subsection 4.4 regarding this aspect.
4. An application: high-frequency behavior through low-frequency asymptotics

At this point, we have generalized Willis theory by using enriched kinematics to improve the quality of approximation of a microscopic displacement $u$ by a macroscopic one $D$. The cost is however the increasing complexity of the resulting effective motion equation. A numerical procedure dedicated to the implementation of Willis’ theory or our previous one is quite heavy, the effective behavior being nonlocal in both space and time with infinite radii of influence in general.

Taylor asymptotic expansions provide an efficient way to approximate the nonlocal behavior with a local one under appropriate assumptions on $k$ and $\omega$. LW-LF expansions have the main advantage of only requiring the solution of static problems but present the disadvantage of being limited to the LF behavior. The purpose of this section is to show explicitly how generalizing Willis theory makes it possible to extend the validity domain of LW-LF expansions to high-frequency behavior over a simple 1D example.

4.1. Setting

Consider the periodically inhomogeneous string whose unit cell is depicted in figure 3, and define the shape function

$$\phi(x) = \sqrt{2} \sin (\pi x / a)$$

which describes the rapidly oscillating body force

$$f = F + q\phi$$
and will carry the new DOF $\chi$. The macroscopic displacement $D$ then reads

$$D = U + \chi \phi$$

with

$$U = \langle u \rangle, \quad \chi = \langle \phi u \rangle.$$
unit cell, the approximate effective impedance $Z$, truncated at order 2 in $k$ and $\omega$, is given by

\[ Z_{UU} = 2 \frac{c_1 c_2}{c_1 + c_2} k^2 - \frac{\rho_1 + \rho_2}{2} \omega^2, \]

\[ Z_{UX} = Z_{XU} = 4 \sqrt{2} \frac{c_1 c_2 (c_1 - c_2)}{\pi (c_1 + c_2)^2} k^2 + \frac{\sqrt{2}}{\pi} (\rho_1 - \rho_2) \omega^2, \]

\[ Z_{XX} = 2 \pi^2 \frac{c_1 c_2}{a^2 (c_1 + c_2)} \]

\[ - \frac{2}{\pi^2} \left[ \left( \pi^2 - 6 \right) \rho_2 + 2 \rho_1 \right] c_1^2 + 4 (\rho_1 + \rho_2) c_1 c_2 + \left( \left( \pi^2 - 6 \right) \rho_1 + 2 \rho_2 \right) c^2 \omega^2 \]

\[ - \frac{2}{\pi^2} \frac{2 c_1 c_2 \left[ \left( 3 \pi^2 - 8 \right) c_1^2 + 2 \left( 3 \pi^2 + 8 \right) c_1 c_2 + \left( 3 \pi^2 - 8 \right) c_2^2 \right]}{(c_1 + c_2)^2} \]

\[ = \bar{F}_k, \]

\[ - 4 \sqrt{2} \frac{c_1 c_2 (c_1 - c_2)}{\pi (c_1 + c_2)^2} \chi'' - \frac{\sqrt{2}}{\pi} (\rho_1 - \rho_2) \chi = F, \]

\[ \chi'' + \frac{\sqrt{2}}{\pi} \left( \rho_1 - \rho_2 \right) \chi + \frac{2 \pi^2}{a^2 (c_1 + c_2)} \frac{c_1 c_2}{(c_1 + c_2)^2} \]

\[ \chi'' + \frac{2 }{\pi^2} \frac{2 c_1 c_2 \left[ \left( 3 \pi^2 - 8 \right) c_1^2 + 2 \left( 3 \pi^2 + 8 \right) c_1 c_2 + \left( 3 \pi^2 - 8 \right) c_2^2 \right]}{(c_1 + c_2)^3} \chi'' = f^w, \]

where a superscripted dot denotes $\partial / \partial t$ and the prime symbol means $\partial / \partial x$. 

In the real domain, the above equation takes the form

\[ \bar{Z}_{k}^{UU} \bar{U}_k + \bar{Z}_{k}^{UX} \bar{\chi}_k = \bar{F}_k, \]

\[ \bar{Z}_{k}^{UX} \bar{U}_k + \bar{Z}_{k}^{XX} \bar{\chi}_k = \bar{q}_k. \]
4.3. Exact and approximate dispersion curves

The expression of the exact dispersion curve is known and was derived elsewhere (Andrianov et al., 2008). It reads:

$$\cos(2ka) = \frac{(\sqrt{c_1\rho_1} + \sqrt{c_2\rho_2})^2}{4\sqrt{c_1\rho_1c_2\rho_2}} \cos \left[ \omega \left( \sqrt{\rho_1/c_1} + \sqrt{\rho_2/c_2} \right) a \right] - \frac{(\sqrt{c_1\rho_1} - \sqrt{c_2\rho_2})^2}{4\sqrt{c_1\rho_1c_2\rho_2}} \cos \left[ \omega \left( \sqrt{\rho_1/c_1} - \sqrt{\rho_2/c_2} \right) a \right].$$

The approximate dispersion curve is derived from the approximate effective impedance according to

$$Z^{UU}Z^{xx} - Z^{xU}Z^{Ux} = 0.$$

The first two branches of the exact and approximate dispersion curves are drawn in figure 4 for the following arbitrary numerical values of the string parameters

$$c_1 = 1, \quad c_2 = 100, \quad \rho_1 = 1, \quad \rho_2 = 5, \quad a = 1.$$

The plots are properly normalized so that units become irrelevant for our purposes. On figure 4, with respect to the classical quasistatic approximation ($\omega_1^{(0)}$), enriching the kinematics allows for capturing the first optical branch and grants a larger validity domain for LF asymptotic expansions. The approximate dispersion branches of order 4 are more precise and almost indistinguishable from the exact ones. The corresponding approximate dispersion relation was numerically found and is not given here. However, we presented the resulting dispersion branches so as to get a glimpse of the convergence rate of the asymptotic scheme. Note that simultaneously capturing additional optical branches requires including richer body forces.
Why is it possible that LF Taylor expansions lead to a correct estimate of some optical modes? Physically speaking, for high frequencies, inertial forces become important and shift the energy carried by displacements toward shorter wavelengths. Correspondingly, including rapidly oscillating body forces have two benefits. First, they simulate the effects of inertial forces. Second, and most importantly, they oblige the macroscopic displacement field to include some short-wavelength components, necessary for approximating the high-frequency behavior. Mathematically speaking, including additional
DOFs delays the appearance of some singularities and extends the convergence domain of the LF Taylor expansions (see Nassar et al., 2015a).

4.4. On the choice of shape functions

The above method and results are by no means universal. Depending on the underlying microstructure and on the targeted frequency range, adequate shape functions can be chosen. Regarding how to appropriately choose shape functions, the following comments are in order:

1. In our 1D example, the sinusoidal shape function was chosen based on considerations similar to the ones arising in Bragg’s reflection where the first term added to the coherent wave is another Fourier component of the exact scattered (microscopic in our terminology) field (see, e.g., Quéré, 1988).

2. In some situations, by inspecting the phases connectedness and contrasts, an asymptotic analysis allows constructing shape functions as particular quasistatic first-order solutions (see, e.g., Auriault and Bonnet, 1985).

3. It can also be proven that including the $n^{\text{th}}$ periodic optical oscillation mode as a shape function guarantees that the $n^{\text{th}}$ optical dispersion branch is correctly approximated at $k = 0$. In fact, this amounts to combining the classical quasistatic homogenization theory with the high-frequency homogenization theory suggested by Daya et al. (2002) and by Craster et al. (2010) and co-workers.

5. Concluding remarks

Through incorporating new kinematical DOFs, the present work has proposed an elastodynamic homogenization theory generalizing the one of Willis
in the case of periodic media and reducing the error committed during the upscaling process, especially at high frequencies. In order to illustrate the potential of the presented theory, it has been shown that the LW-LF asymptotic expansion of the effective motion equation is capable of simultaneously capturing the acoustic and the first optical branch of the microscopic dispersion curve for a simple 1D medium.

Two problems remain open. The first concerns the effective elastodynamic constitutive law produced by the generalized theory proposed. In this paper, to avoid the difficulty related to its non-uniqueness, the effective motion equation has been directly treated and exploited. However, in numerous situations, it is useful and important to explicitly know the effective elastodynamic constitutive law. The second problem regards the optimal choice of shape functions for which guiding criteria exist but remain incomplete.

References


Auriault, J.L., Bonnet, G., 1985. Dynamics of periodic elastic composites


