The response of linear inhomogeneous systems to coupled fields: Bounds and perturbation expansions

Mordehai Milgrom* and Graeme W. Milton**

*Department of Particle Physics and Astrophysics, Weizmann Institute of Science, 76100 Rehovot, Israel
**Department of Mathematics, University of Utah, Salt Lake City, UT 84112, USA
emails: moti.milgrom@weizmann.ac.il, milton@math.utah.edu

Abstract

We consider the response of a multicomponent body to $n$ fields, such as electric fields, magnetic fields, temperature gradients, concentration gradients, etc., where each component, which is possibly anisotropic, may cross couple the various fields with different fluxes, such as electrical currents, electrical displacement currents, magnetic induction fields, energy fluxes, particle fluxes, etc. We obtain the form of the perturbation expansions of the fields and response tensor in powers of matrices which measure the difference between each component tensor and a homogeneous reference tensor $L_0$. For the case of a statistically homogeneous or periodic composite the expansion coefficients can be expressed in terms of positive semidefinite normalization matrices alternating with positive semidefinite weight matrices, which at each given level sum to the identity matrix. In an appropriate basis the projection operators onto the relevant subspaces can be expressed in block tridiagonal form, where the blocks are functions of these weight and normalization matrices. This leads to continued fraction expansions for the effective tensor, and by truncating the continued fraction at successive levels one obtains a nested sequence of bounds on the effective tensor incorporating successively more weight and normalization matrices. The weight matrices and normalization matrices can be calculated from the series expansions of the fields which solve the conductivity problem alone, without any couplings to other fields, and then they can be used to obtain the solution for the fields and effective tensor in coupled field problems in composites.

1 Introduction

This Chapter 9 of the book "Extending the Theory of Composites to other Areas of Science", edited by Graeme W. Milton, is concerned with the response of coupled fields and fluxes in a three-dimensional body $\Omega$ to potentials prescribed at the boundary of the body and with how this response depends on the material constants of the body. The effective tensor of a statistically homogeneous or periodic composite, with coupling between the fields, is a special case which we will study in more depth. The set of fields $\vec{E} = (\vec{E}_1, \vec{E}_2, ..., \vec{E}_n)$ which are each curl-free, may include electric fields, magnetic fields, temperature gradients, or concentration gradients and the associated fluxes $\vec{J} = (\vec{J}_1, \vec{J}_2, ..., \vec{J}_n)$ may include electrical currents, electrical displacement currents, magnetic induction fields, energy fluxes and particle fluxes. We assume there are no sources inside the body, so each of these fluxes is divergence free. Assuming a simply connected topology of the body, each of the curl-free fields derive from a potential $\vec{E}_j = -\nabla \phi^j$.

At each point within the body or medium we assume a linear constitutive relation $\vec{J} = \hat{L} \vec{E}$ between the fluxes and fields through a position dependent symmetric positive-definite tensor
\(\mathbf{T}(\mathbf{r})\) of material constants. The tensor may have off-diagonal couplings which cause a single driving field, such as a temperature gradient, to induce fluxes of all types.

The body is assumed to be an aggregate of grains (possibly infinite in number) comprised of a finite number \(M\) of components (phases) that have at least orthorhombic symmetry with the crystal orientation varying from grain to grain, thus \(\mathbf{T}(\mathbf{r})\) is assumed to be piecewise constant. Let \(\mathbf{L}_{l}\alpha, \ l = 1, 2, \ldots M, \ \alpha = 1, 2, 3\) be the \(n \times n\) principal response matrices of the \(l\)-th component, defined more precisely in the next Section.

We investigate the response of the set of fluxes, \(\mathbf{J}(\mathbf{r})\), measured at a given position \(\mathbf{r}\) within the body, to the potentials \(\phi(\mathbf{r}) = [\phi^1(\mathbf{r}), \ldots, \phi^n(\mathbf{r})]\) prescribed at the boundary of the body. Without loss of generality (see Milgrom (1990) for a discussion of this point) it is assumed that the prescribed potentials are all in proportion to a fixed scalar function \(f(\mathbf{r})\) defined at points \(\mathbf{r}\) on the surface of the body, i.e. \(\phi^i(\mathbf{r}) = \phi^0 f(\mathbf{r})\) for all \(\mathbf{r} \in \partial \Omega\), and we consider how the set of fluxes \(\mathbf{J}(\mathbf{r})\) at \(\mathbf{r}\) vary with the choice of the vector \(\phi_0 = (\phi^1_0, \ldots, \phi^n_0)\) of proportionality constants: since this relation is linear it is governed by a response tensor \(\mathbf{L}(\mathbf{r})\) giving \(\mathbf{J}(\mathbf{r}) = \mathbf{L}(\mathbf{r})\phi_0\). This tensor \(\mathbf{L}(\mathbf{r})\) is the object of our analysis. Specifically we examine the dependence of \(\mathbf{L}(\mathbf{r})\) on the set of crystal moduli \(\mathbf{L}_{l}\alpha\) \((l = 1, 2, \ldots M, \alpha = 1, 2, 3)\) when each is close to a constant tensor \(\mathbf{L}_0\), i.e. when the material constants of the body are close to being homogeneous and isotropic. To simplify notations these crystal moduli are relabeled as \(\mathbf{L}_a\) \((a = 1, 2, \ldots, p)\), avoiding repetitions in the original set of crystal moduli due to crystal symmetries of isotropy or uniaxiality: thus, when there are no symmetries (other than orthorhombic symmetry) \(a\) represents the pair \((l, \alpha)\) and \(p = 3M\), but \(p\) could be less than \(3M\) if some of the phases are isotropic or uniaxial.

A formal expression is obtained for the coefficients appearing in the series expansion of \(\mathbf{L}(\mathbf{r})\) in powers of the differences \(\epsilon_a = \mathbf{L}_a - \mathbf{L}_0\) \((a = 1, 2, \ldots, p)\). We say formal because these coefficients are difficult to evaluate and because their (nonlinear and nonlocal) dependence on the overall shape of the body, on the division of the body into grains and on the orientation of the crystals in each grain is complicated. What is interesting is the explicit form of the expansion. This is a non trivial issue since the set of matrices \(\mathbf{L}_a\) \((a = 1, 2, \ldots, p)\) do not necessarily commute. The issue has been addressed in part by Milgrom (1990) from general analytic considerations. Milgrom noted that the functional dependence of \(\mathbf{L}(\mathbf{r})\) on the \(\mathbf{L}_a\) must satisfy two constraints:

(i) **Covariance**, the property that for any real, nonsingular, \(n\) by \(n\) matrix \(\mathbf{W}\) with transpose \(\mathbf{W}^T\) acting only on the field indices, the response tensor \(\mathbf{L}(\mathbf{r})\) transforms to \(\mathbf{W}^T \mathbf{L}(\mathbf{r}) \mathbf{W}\) when all of the crystal moduli \(\mathbf{L}_a\) are replaced by the moduli \(\mathbf{W} \mathbf{L}_a \mathbf{W}^T\). Covariance follows from the observation that we are free to define a new set of (curl-free) fields \(\mathbf{E}' = (\mathbf{W}^T)^{-1} \mathbf{E}\) and a new set of (divergence-free) fluxes \(\mathbf{J}' = \mathbf{W}^T \mathbf{J}\) by taking linear combinations of the old set of fields and fluxes while preserving at the same time the self-adjointness of the tensor \(\mathbf{L}(\mathbf{r}) = \mathbf{W}^T \mathbf{L}(\mathbf{r}) \mathbf{W}\) in the constitutive relation \(\mathbf{J}' = \mathbf{L}' \mathbf{E}\). Clearly \(\mathbf{W}^T \mathbf{L}(\mathbf{r}) \mathbf{W}\) is simply the old response tensor \(\mathbf{L}(\mathbf{r})\) expressed in terms of the new fields.

(ii) **Disjunction**, the property that when the matrices \(\mathbf{L}_a\) are block diagonal of the same form then so must \(\mathbf{L}(\mathbf{r})\) have a similar block diagonal form in the field indices, and furthermore the elements of \(\mathbf{L}(\mathbf{r})\) within each block only depend on the elements of the \(\mathbf{L}_a\)’s in the corresponding blocks. Disjunction follows from the observation that if a subset of fields is decoupled from another subset of fields then the effective response tensor must reflect this decoupling.

These analytic considerations alone eliminate from consideration many candidates for the terms in the series expansion, such as for example \(\mathbf{L}_0^{-1} \epsilon_{a_1} \epsilon_{a_2}\), and leave terms such as \(\epsilon_{a_1} \mathbf{L}_0^{-1} \epsilon_{a_2} \mathbf{L}_0^{-1} \epsilon_{a_3}\) (that in fact do occur in the series expansion) as natural candidates.

The technique we employ in the present Chapter is a simple generalization of an approach used in the theory of composite materials to derive series expansions for the effective conductiv-
ity or elasticity tensor of a nearly homogeneous multiphase material. A lot of the progress that has been made on series expansions and associated bounds on effective tensors is summarized in the books of Cherkaev (2000), Milton (2002), Allaire (2002), Torquato (2002), Tartar (2009), Brown (1955), in a pioneering paper, obtained the series expansion of the effective conductivity \( \sigma^* \) of an isotropic composite of two isotropic components with nearly equal conductivities \( \sigma_1 \) and \( \sigma_2 \), and found that the coefficient of \( (\sigma_1 - \sigma_2)^n \) in this expansion depends on the \( n \)-point correlation function giving the probability that a fixed configuration of \( n \)-points lands with all points in component 1 when placed randomly in the composite. Subsequently many other series expansions were derived for the effective conductivity tensor or elasticity tensor of nearly homogeneous composites: see for example, Herring (1960), Prager (1960), Beran and Molyneux (1963), Beran (1968), Beran and McCoy (1970), Fokin and Shemerger (1969), Dederichs and Zeller (1973), Hori (1973), Zeller and Dederichs (1973), Gubernatis and Krumhansl (1975), Kröner (1977), Willis (1981), Milton and Phan-Thien (1982), Sen and Torquato (1989), Torquato (1997), Tartar (1989, 1990), and Bruno (1991). Our analysis closely follows that of Willis (1981) and Phan-Thien and Milton (1982, 1983).

Our analysis gives, as a simple corollary, a series expansion for the effective tensor \( \mathbf{L}^* \) that governs the constitutive relation between the local average of \( \mathbf{J} \) and the local average of \( \mathbf{E} \) in a statistically homogeneous or periodic composite material. (These averages are taken over a length scale much larger than the microstructure, yet smaller than any macroscopic lengths associated with variations in the applied fields.) This expansion is derived in Section 4 where the body is assumed to be filled with such a composite material, with microstructure much smaller than the dimensions of the body. From the response tensor \( \mathbf{L}(\mathbf{r}) \) associated with linear potentials specified on the boundary, i.e. with \( f(\mathbf{r}) = -\mathbf{r} \cdot \mathbf{v}_0 \) on \( \partial \Omega \), where \( \mathbf{v}_0 \) gives the direction of the applied field, we directly obtain the effective tensor \( \mathbf{L}^* \) of the composite.

The coefficients in the series expansion of \( \mathbf{L}^* \) in powers of the \( \mathbf{e}_a \) \((a = 1, 2, \ldots, p) \) are useful for obtaining bounds on \( \mathbf{L}^* \). In particular they likely contain sufficient information to determine the weight and normalization matrices that were introduced by Milton (1987a, 1987b), following the introduction of scalar valued weights and normalization factors by Milton and Golden (1985). Thus these parameters are seen to have a natural significance in the context of coupled field problems. In any case the weight matrices and normalization matrices can be calculated from the series expansions of the fields. It is noteworthy that they can be calculated from the series expansions of the fields which solve the conductivity problem alone, without any couplings to other fields, and then they can be used to obtain the solution for the fields and effective tensor \( \mathbf{L}^* \) in coupled field problems.

With these geometric parameters we show how one can compute, for coupled field problems, the Wiener-Beran and Hashin-Shtrikman type bounds of any order: these bounds, derived for the effective conductivity by Milton (1981) and Milton and McPhedran (1982) (see also McPhedran and Milton 1981) and extended here to bounds on \( \mathbf{L}^* \), generalize the bounds of Wiener (1912), Hashin and Shtrikman (1962), Beran (1965), Willis (1977), Phan-Thien and Milton (1982), and Sen and Torquato (1989). They do not, however, encompass the optimal two-dimensional, two-phase bounds of Cherkaev and Gibiansky (1992) and Clark and Milton (1995) which couple effective tensors using additional information about the differential constraints on the fields, or duality relations satisfied by the effective tensor as a function of the component moduli. Again many of the existing bounds are summarized in the books of Cherkaev (2000), Milton (2002), Allaire (2002), Torquato (2002), Tartar (2009).
2 Setting of the problem and equations for the fields

We consider the problem of linear response to \( n \) coupled fields derivable from potentials \( \phi^k \), \( k = 1, \ldots, n \). The problem is described, in detail, by Milgrom (1990), and we give a succinct description here. The body consists of a space domain \( \Omega \) within which the position-dependent response tensor is \( L_{\alpha i\beta k}(\vec{r}) \), where \( i, k \) are field indices and \( \alpha, \beta \) are space indices. The \( \alpha \)th component of the \( i \)th flux is given by the constitutive relation

\[
J_i^\alpha(\vec{r}) = -\sum_{k=1}^{n} \sum_{\beta=1}^{3} L_{\alpha i\beta k}(\vec{r}) \partial_\beta \phi^k(\vec{r}),
\]

or, suppressing the indices:

\[
\vec{J} = -\vec{L} \vec{\nabla} \phi.
\]

We shall be using boldface letters for quantities that are vectors or tensors in the field indices. Also, \( \rightarrow \) above a character indicates a vector in the space indices and \( \leftrightarrow \) above a character indicates a matrix in the space indices. So, for example, \( \vec{J}, \vec{E}, \) and \( \vec{\epsilon} \) are vectors in both space and field indices; \( \vec{L}, \) and \( \vec{\epsilon} \) are second rank tensors in both types of indices; \( L \) is a matrix in the field indices; \( \phi \) and \( \phi_0 \) are vectors in the field indices; \( \vec{r} \) is a vector in the space indices; and \( \vec{\Gamma}_1 \) is a matrix in the space indices.

The equation

\[
\vec{\nabla} \cdot \vec{J} = 0,
\]

determines the fields \( \phi \) within \( \Omega \), given the boundary conditions.

The response we consider is the field vector of \( n \) fluxes, \( \vec{J}(\vec{r}) \), measured at a given position \( \vec{r} \) within \( \Omega \), and is taken to respond to the boundary conditions dictated on the surface, \( \partial \Omega \), of \( \Omega \). As explained in Milgrom (1990), we may, without loss of generality, restrict ourselves to boundary conditions of the form

\[
\phi(\vec{r}) = \phi_0 f(\vec{r}), \quad \vec{r} \in \partial \Omega.
\]

We then define the response matrix \( \vec{L}(\vec{r}) \) such that

\[
\vec{J}(\vec{r}) = \vec{L}(\vec{r}) \phi_0.
\]

We shall be interested in a piecewise-homogeneous system, so \( \Omega \) is divided into a (possibly infinite) number of domains, as in Fig. 1, each of which is filled with one of \( M \) (possibly anisotropic) components, with an arbitrary orientation of its axes. We restrict ourselves to components that have, at least, an orthorhombic symmetry. The response matrix, \( \vec{L}(\vec{r}) \), depends, then, on the shape of \( \Omega \), on the choice of \( f(\vec{r}) \), on the division of \( \Omega \) into sub-domains, on the orientations of the different components within these homogeneous sub-domains, and on the response properties of the individual components. In the principal axes of the \( l \)th component we can write

\[
L_{\alpha k\beta m}^l = L_{km}^{l,\alpha} \delta_{\alpha\beta},
\]

where there is no summation over \( \alpha \) and the \( L_{km}^{l,\alpha} \) \( (\alpha = 1, 2, 3) \) are the principal response matrices of component \( l, \ l = 1, 2, \ldots, M \). Let \( p \) be the total number of such principal matrices characterizing all the components. So, there is only one such matrix for an isotropic component, two for a component with uniaxial symmetry, and three for a component with orthorhombic symmetry. We shall use a single index notation with \( L_a, \ a = 1, \ldots, p \) instead of the doubly indexed \( L_{km}^{l,\alpha} \). (Depending on the symmetry, \( \alpha \) here takes one, two, or three values.)
In the isotropic and homogeneous case we have
\[ L_a = L_0, \]  
(2.7)
for all \( a \). When there are departures from isotropy and homogeneity we write
\[ L_a = L_0 + \epsilon_a, \]  
(2.8)
and seek to expand \( \vec{E}(\vec{r}) \) in the elements \( \epsilon_{ik}^a \) of the \( \epsilon_a \)'s.

To this end we first derive a formal expression for the driving field, \( \vec{E} = -\vec{\nabla}\phi \) produced within \( \Omega \) by the boundary conditions \( \phi_0 \). Let \( \vec{E}_0 \) be the driving field that is produced by these same boundary conditions in the homogeneous, isotropic case. We can write
\[ \vec{E}_0(\vec{r}) = \phi_0 \vec{v}_0(\vec{r}), \]  
(2.9)
where \( \vec{v}_0 = -\vec{\nabla}\psi_0 \), and \( \psi_0 \) is the single-field solution of the Laplace equation, in \( \Omega \), with boundary condition \( \psi(\vec{r}) = f(\vec{r}) \) on \( \partial\Omega \); thus \( \vec{\nabla} \cdot \vec{E}_0 = 0 \). The difference field
\[ \vec{e} \equiv \vec{E} - \vec{E}_0 = -\vec{\nabla}\psi, \]  
(2.10)
is derivable from a potential \( \psi \), that vanishes on \( \partial\Omega \). Now introduce
\[ \vec{\Gamma}(\vec{r}) = \vec{L}(\vec{r}) - L_0 \hat{I}, \]  
(2.11)
where we use \( \hat{I} \) for the unit matrix in space indices; \( \hat{I} \) for the identity in both space and field indices; and \( I \) for the identity operator which when acting on a function leaves it invariant. Then the flux field,
\[ \vec{J}(\vec{r}) = \vec{L}(\vec{r})\vec{E}(\vec{r}), \]  
(2.12)
can thus be written as
\[ \vec{J}(\vec{r}) = [L_0 \hat{I} + \vec{\epsilon}(\vec{r})](\vec{E}_0 + \vec{e})(\vec{r}). \]  
(2.13)
Taking the divergence of (2.13), and remembering that \( \vec{J} \) and \( L_0\vec{E}_0 \) are divergence-free, we obtain
\[ L_0\vec{\nabla} \cdot \vec{e} + \vec{\nabla} \cdot (\vec{\epsilon} \vec{E}) = 0, \]  
(2.14)
or equivalently,
\[ \Delta \psi = \vec{\nabla} \cdot (L_0^{-1}\vec{\epsilon} \vec{E}). \]  
(2.15)
Define, now, the inverse-Laplacian, \( \Delta^{-1} \), as the nonlocal operator which, acting on a density function \( \rho(\vec{r}) \), defined in \( \Omega \), gives the potential \( \varphi \) that solves the Poisson’s equation \( \Delta \varphi = -\rho \), and vanishes on the surface, \( \partial\Omega \). Then, from (2.15) and (2.10) we can write
\[ \vec{e} = -\vec{\Gamma}_1 L_0^{-1}\vec{\epsilon} \vec{E}, \]  
(2.16)
where
\[ \vec{\Gamma}_1 \equiv \vec{\nabla} \Delta^{-1} \vec{\nabla}, \]  
(2.17)
is nonlocal, with kernel \( \vec{\Gamma}_1(\vec{r}, \vec{r}') \), and acts on a vector field \( \vec{u}(\vec{r}') \) to give the vector field
\[ \vec{v}(\vec{r}) = \int_\Omega d\vec{r}' \vec{\Gamma}_1(\vec{r}, \vec{r}') \vec{u}(\vec{r}'), \]  
(2.18)
that has the same divergence as \( \vec{u} \), and is derivable from a potential that vanishes on \( \partial\Omega \). Clearly, \( \vec{\Gamma}_1 \) is a projection operator:
\[ \vec{\Gamma}_1 \vec{\Gamma}_1 = \vec{\Gamma}_1, \]  
(2.19)
implying its kernel satisfies
\[ \Gamma_1(\vec{r},\vec{r}') = \int_\Omega d\vec{r}'' \Gamma_1(\vec{r},\vec{r}'') \Gamma_1(\vec{r}'',\vec{r}'). \]  

(2.20)

In addition, because \( \Gamma_1 \) gives zero when it acts on a uniform vector field and always produces a vector field with zero integral over \( \Omega \), we have
\[ \int_\Omega d\vec{r}' \Gamma_1(\vec{r},\vec{r}') = 0, \quad \int_\Omega d\vec{r} \Gamma_1(\vec{r},\vec{r}') = 0. \]  

(2.21)

The operator \( \Gamma_1 \) is also self-adjoint, i.e.
\[ \Gamma_1(\vec{r},\vec{r}') = [\Gamma_1(\vec{r}',\vec{r})]^T, \]  

(2.22)

where \( T \) denotes the transpose. To see this, suppose one is given vector fields \( \vec{u}(\vec{r}) \) and \( \vec{v}(\vec{r}) \). Let \( \phi(\vec{r}) \) and \( \psi(\vec{r}) \) be potentials that vanish on the boundary \( \partial \Omega \) such that
\[ \vec{u} = \vec{\nabla} \phi + \vec{\nabla} \times \vec{A}, \quad \vec{v} = \vec{\nabla} \psi + \vec{\nabla} \times \vec{B}, \]  

(2.23)

for some vector potentials \( \vec{A}(\vec{r}) \) and \( \vec{B}(\vec{r}) \). Then the definition of \( \Gamma_1 \) implies \( \Gamma_1 \vec{u} = \vec{\nabla} \phi \) and \( \Gamma_1 \vec{v} = \vec{\nabla} \psi \). So we have
\[ \int_\Omega \vec{v} \cdot (\vec{\Gamma}_1 \vec{u}) = \int_\Omega \vec{\nabla} \psi \cdot \vec{\nabla} \phi + \int_\Omega (\vec{\nabla} \times \vec{B}) \cdot \vec{\nabla} \phi. \]  

(2.24)

Using the divergence theorem, the last integral vanishes,
\[ \int_\Omega (\vec{\nabla} \times \vec{B}) \cdot \vec{\nabla} \phi = \int_\Omega \vec{\nabla} \cdot [\phi(\vec{\nabla} \times \vec{B})] = \int_{\partial \Omega} \phi \cdot (\vec{\nabla} \times \vec{B}) = 0, \]  

(2.25)

where \( \vec{n} \) is the outwards normal to \( \partial \Omega \), and we have used the fact that \( \phi = 0 \) on \( \partial \Omega \). Switching the roles of \( \vec{v} \) and \( \vec{u} \) in (2.24) gives the same result, and so we obtain
\[ \int_\Omega \vec{v} \cdot (\vec{\Gamma}_1 \vec{u}) = \int_\Omega \vec{u} \cdot (\vec{\Gamma}_1 \vec{v}), \]  

(2.26)

which means \( \vec{\Gamma}_1 \) is self-adjoint.

Adding \( \vec{E}_0 \) to both sides of (2.16), we can write
\[ (I + \vec{\Gamma}_1 \vec{L}_0^{-1}) \vec{E} = \vec{E}_0, \]  

(2.27)

or
\[ \vec{E} = (I + \vec{\Gamma}_1 \vec{L}_0^{-1})^{-1} \vec{E}_0. \]  

(2.28)

Thus, from the definition of the response matrix \( \vec{L}(\vec{r}) \), equation (2.5), from relation (2.9) between \( \vec{E}_0 \) and \( \vec{\phi}_0 \), and from relation (2.12) between \( \vec{J} \) and \( \vec{E} \), we get
\[ \vec{L}(\vec{r}) = \int d\vec{r}' \vec{S}(\vec{r},\vec{r}') \vec{v}_0(\vec{r}'), \]  

(2.29)

where \( \vec{S}(\vec{r},\vec{r}') \) is the kernel of a nonlocal operator \( \vec{S} \) [acting on the field \( \vec{v}_0 \)], given by
\[ \vec{S} = (\vec{L}_0 \Gamma + \vec{\epsilon})(I + \vec{\Gamma}_1 \vec{L}_0^{-1})^{-1}. \]  

(2.30)

The vector field \( \vec{v}_0 \) only carries the information on the exact form of the boundary conditions \( [f(\vec{r}_0)] \); it is \( \vec{S}(\vec{r},\vec{r}') \) that plays the role of the response tensor of the system.
We now use (2.30) to develop a series expansion for the response tensor \( \mathbf{S}(\vec{r}, \vec{r}') \). Specializing to the piecewise homogeneous case, we express \( \mathbf{e}(\vec{r}) \) in terms of the \( \epsilon_a \)'s defined in equation (2.8). Defining the indicator function, \( \chi_l(\vec{r}) \), such that \( \chi_l(\vec{r}) = 1 \) in a subregion occupied by component \( l, l = 1, 2, \ldots, M \) and \( \chi_l(\vec{r}) = 0 \) otherwise, we can write for the \( \alpha\beta \) element of \( \mathbf{e} \)

\[
\epsilon_{\alpha\beta}(\vec{r}) = \sum_{l=1}^{M} \sum_{\eta=1}^{3} \chi_l(\vec{r}) R_{\alpha\eta}(\vec{r}) \epsilon^{\eta}\epsilon^{\eta T}(\vec{r}), \tag{3.1}
\]

where

\[
\epsilon^{\eta} = L^{\eta} - L_0, \tag{3.2}
\]

and \( L^{\eta} \) are the principal response matrices of component \( l \), \( R(\vec{r}) \) is the rotation matrix from the principal axes to the orientation the component has at position \( \vec{r} \), and \( R^T(\vec{r}) \) is its transpose (inverse).

Equation (3.1) can be cast in the form

\[
\epsilon_{\alpha\beta}(\vec{r}) = \sum_{a=1}^{p} \Lambda_{a,\alpha\beta}(\vec{r}) \epsilon_a, \tag{3.3}
\]

where the elements, \( \Lambda_{a,\alpha\beta}(\vec{r}) \), of \( \mathbf{\Lambda}_a \) are defined as follows: For an orthorhombic component, there are three \( \mathbf{\Lambda}_a \)'s, where \( a \) replaces the double index \( l, \eta \), and

\[
\Lambda_{\alpha\beta}^{L,\eta}(\vec{r}) = \chi_l(\vec{r}) R_{\alpha\eta}(\vec{r}) R_{\eta\beta}^{T}(\vec{r}) \tag{3.4}
\]

(with no summation over \( \eta \)). When the component \( l \) is isotropic, it contributes only one \( \mathbf{\Lambda}_a \), with

\[
\Lambda_{\alpha\beta}^a(\vec{r}) = \chi_l(\vec{r}) \sum_{\eta=1}^{3} R_{\alpha\eta}(\vec{r}) R_{\eta\beta}^{T}(\vec{r}) = \chi_l(\vec{r}) \delta_{\alpha\beta}. \tag{3.5}
\]

Similarly, for a uniaxial component there are two matrices \( \mathbf{\Lambda}_a(\vec{r}) \). It is easy to ascertain that

\[
\mathbf{\Lambda}_a(\vec{r}) \mathbf{\Lambda}_b(\vec{r}) = \delta_{ab} \mathbf{\Lambda}_a(\vec{r}), \tag{3.6}
\]

and we also have

\[
\sum_{a=1}^{p} \mathbf{\Lambda}_a(\vec{r}) = \mathbf{\Lambda} \tag{3.7}
\]

Now, substituting (3.3) in expression (2.30) for \( \mathbf{\hat{S}} \), and expanding, we get

\[
\mathbf{\hat{S}} = L_0 \mathbf{\hat{I}} + \sum_{s=1}^{\infty} \sum_{a_1, \ldots, a_s=1} \epsilon_{a_1} L_0^{-1} \epsilon_{a_2} L_0^{-1} \ldots L_0^{-1} \epsilon_{a_s}, \tag{3.8}
\]

where the reduced operator \( \mathbf{\hat{K}}_{a_1 \ldots a_s} \) is given by

\[
\mathbf{\hat{K}}_{a_1 \ldots a_s} = (I - \mathbf{\Gamma}_1) \mathbf{\hat{A}}_{a_1} \mathbf{\hat{A}}_{a_2} \mathbf{\hat{A}}_{a_3} \ldots \mathbf{\hat{A}}_{a_s}. \tag{3.9}
\]

Note that each operator \( \mathbf{\hat{A}} \) in the above relation acts on the whole expression to its right including the field on which \( \mathbf{\hat{K}}_{a_1 \ldots a_s} \) acts: it does not just act on the adjacent \( \mathbf{\Lambda}_a(\vec{r}) \) factor.
The reduced operators, which are matrices in the space indices, are purely geometrical. They depend on the geometry of the region $\Omega$, on its division into homogeneous sub-regions, and on the orientation of the components within these sub-regions. They do not depend on the form of the boundary condition $f(\vec{r}_0)$, which enter through $\vec{v}_0(\vec{r})$ (on which the $\vec{K}$’s act); they also do not depend on the response coefficients of the components, which enter through the field-matrix terms in (3.8).

Using (2.29), the corresponding reduced, expansion coefficients of the response $\vec{L}(\vec{r})$ are

$$\vec{\kappa}_{a_1...a_s}(\vec{r}) = [\vec{K}_{a_1...a_s} \vec{v}_0](\vec{r}) = \int_{\Omega} d\vec{r}' \vec{K}_{a_1...a_s}(\vec{r}, \vec{r}') \vec{v}_0(\vec{r}'),$$

where $\vec{K}_{a_1...a_s}(\vec{r}, \vec{r}')$ is the kernel of the operator $\vec{K}_{a_1...a_s}$. Note that the reduced coefficients are not independent: Summing over the last index gives

$$\sum_{a_s=1}^{p} \vec{\kappa}_{a_1...a_s} = 0,$$

from (3.7), and the fact that $\vec{\Gamma}_1$ acting on a divergence-free vector field (such as $\vec{v}_0$) gives 0. Summing over the first index we also have

$$\sum_{a_1=1}^{p} \vec{\kappa}_{a_1...a_s} = 0,$$

because $(I - \vec{\Gamma}_1)^\dagger \vec{\Gamma}_1 = 0$. Summing over any, but the last, or first, index gives a reduced coefficient with one less index:

$$\sum_{a_1=1}^{p} \vec{\kappa}_{a_1...a_s} = \vec{\kappa}_{a_1...a_{i-1}a_{i+1}...a_s}.$$

These follow directly from (3.9), and stem from the fact that we could arbitrarily redefine $L_0$ by adding to it a constant matrix, and subtract that matrix from the $\epsilon_a$’s, without affecting $\vec{S}(\vec{r}, \vec{r}')$. So there are really only $(p - 1)^s$ independent $s$-th order coefficients, not $p^s$.

4 The expansion of the effective tensor of a composite

We now focus attention on an important subclass of inhomogeneous bodies: those filled with a statistically homogeneous or periodic composite material with microstructure much smaller than the dimensions of the body. It is well-known and can be rigorously proved (see for example Golden and Papanicolaou (1983)) that if there exists an intermediate length scale $\lambda$ much larger than the homogeneities yet much smaller than the length scales associated with the dimensions of $\Omega$ and with variations in the applied potentials, then $\vec{L}(\vec{r})$ can be replaced by a constant effective tensor $L^*$ without disturbing the macroscopic response of the body. At distances from the boundary $\partial \Omega$, inside the body, sufficiently greater than $\lambda$ this effective tensor $L^*$ governs the relation between the fields

$$< \vec{J} >_{\Theta(\vec{r})} = \frac{1}{|\Theta(\vec{r})|} \int_{\Theta(\vec{r})} d\vec{r}' \vec{J}(\vec{r}'),< \vec{E} >_{\Theta(\vec{r})} = \frac{1}{|\Theta(\vec{r})|} \int_{\Theta(\vec{r})} d\vec{r}' \vec{E}(\vec{r}'),$$

obtained by averaging $\vec{J}(\vec{r}')$ and $\vec{E}(\vec{r}')$ over a sphere $\Theta(\vec{r})$ of volume $|\Theta(\vec{r})|$, centered at $\vec{r}$, with radius $\lambda$, through the constitutive relation

$$< \vec{J} >_{\Theta(\vec{r})} = L^* < \vec{E} >_{\Theta(\vec{r})}.$$
Another tensor of interest is the microscopic response tensor \( \mathbf{L}(\vec{r}', \vec{r}) \) which governs the linear relation between \( \vec{J}(\vec{r}') \) for points \( \vec{r}' \) in \( \Theta(\vec{r}) \), and \( \left< \vec{E} \right>_{\Theta(\vec{r})} \):

\[
\vec{J}(\vec{r}) = \mathbf{L}(\vec{r}', \vec{r}) \left< \vec{E} \right>_{\Theta(\vec{r})} . \tag{4.3}
\]

This tensor \( \mathbf{L}(\vec{r}', \vec{r}) \) is only well-defined if there is a sufficient separation of length scales so that homogenization theory (see the many references in the introduction in Chapter 1 of this book, “Extending the Theory of Composites to Other Areas of Science” edited by Graeme W. Milton, and in particular Bensoussan, Lions, and Papanicolaou 1978 and Kozlov 1978) applies. Then \( \mathbf{L}(\vec{r}', \vec{r}) \) is independent of the choice of \( f(\vec{r}_0) \) (subject to it being smooth and only varying on the macroscopic scale), on the choice of \( \phi_0 \), and (assuming statistical homogeneity) on the value of \( \vec{r} \). Then we may vary \( f(\vec{r}_0) \) and \( \phi_0 \) to change \( \left< \vec{E} \right>_{\Theta(\vec{r})} \) and thus determine \( \mathbf{L}(\vec{r}', \vec{r}) = \mathbf{L}(\vec{r}') \) through (4.3). For materials that are periodic inside \( \Omega \), with periodic cell much smaller than the size of \( \Omega \), \( \mathbf{L}(\vec{r}') \) can be obtained from the fields that solve the homogenization cell problem, i.e. with \( \vec{J}(\vec{r}) \) and \( \vec{E}(\vec{r}) \) having the same periodicity as the material, and the cell average of \( \vec{E}(\vec{r}) \) having any value we desire.

By assumption \( \left< \vec{E} \right>_{\Theta(\vec{r})} \) has a smooth dependence on \( \vec{r} \) and so by taking the average of (4.3) over points \( \vec{r}' \) in the sphere \( \Theta(\vec{r}) \) we can identify \( \mathbf{L}^* \) with the average of \( \mathbf{L}(\vec{r}') \),

\[
\mathbf{L}^* = \left< \mathbf{L} \right>_{\Theta(\vec{r})} = \frac{1}{|\Theta(\vec{r})|} \int_{\Theta(\vec{r})} d\vec{r}' \mathbf{L}(\vec{r}') . \tag{4.4}
\]

To determine \( \mathbf{L}(\vec{r}) \) and hence \( \mathbf{L}^* \) it suffices to prescribe linear potentials on the boundary \( \partial \Omega \) of \( \Omega \), i.e. to suppose \( f(\vec{r}_0) \) takes the form

\[
f(\vec{r}_0) = -\vec{r}_0 \cdot \vec{v}_0 , \tag{4.5}
\]

where \( \vec{v}_0 \) is a constant vector. Then the fields \( \vec{E}_0 \) and \( \left< \vec{E} \right>_{\Theta(\vec{r})} \) which solve the constitutive equations in a homogeneous body are uniform,

\[
\vec{E}_0 = \left< \vec{E} \right>_{\Theta(\vec{r})} = \vec{v}_0 \phi_0 . \tag{4.6}
\]

Consequently for the purpose of determining both \( \mathbf{L}(\vec{r}') \) and \( \mathbf{L}^* \) the averages \( < \left< \vec{E} \right>_{\Theta(\vec{r})} > \) over each sphere \( \Theta(\vec{r}) \) can be replaced by averages \( < \left< \vec{E} \right>_{\Omega} > \) over the entire body \( \Omega \). Also to simplify subsequent formula let us select our dimensions of length so that the body has unit volume,

\[
|\Omega| = 1 . \tag{4.7}
\]

Then, averages over \( \Omega \) can be equated with integrals over \( \Omega \). From (4.6) and the relations (2.5) and (4.3) of \( \mathbf{L}(\vec{r}') \) and \( \mathbf{L}(\vec{r}') \) we have

\[
\mathbf{L}(\vec{r}) = \left< \mathbf{L} \right>(\vec{r}) \vec{v}_0 . \tag{4.8}
\]

where we have relabelled \( \vec{r}' \) as \( \vec{r} \) to avoid confusion in the subsequent formulae. This, in conjunction with (2.29) and (4.4), leads directly to the expressions

\[
\mathbf{L}(\vec{r}) = \int_{\Omega} d\vec{r}' \mathbf{S}(\vec{r}, \vec{r}') , \tag{4.9}
\]

\[
\mathbf{L}^* = \int_{\Omega} d\vec{r} \int_{\Omega} d\vec{r}' \mathbf{S}(\vec{r}, \vec{r}') , \tag{4.10}
\]

9
for the microscopic response tensor $\hat{\mathbb{L}}(\vec{r})$ and the effective tensor $\hat{\mathbb{L}}^*$. Substitution of the series expansion for $\hat{\mathbb{S}}(\vec{r}, \vec{r}')$ into these expressions gives the desired series expansions

$$\hat{\mathbb{L}}(\vec{r}) = L_0 \hat{I} + \sum_{s=1}^{\infty} \sum_{a_1, \ldots, a_s=1}^P (-1)^{s+1} \hat{\mathbb{A}}_{a_1 \ldots a_s} \epsilon_{a_1} L_0^{-1} \epsilon_{a_2} L_0^{-1} \ldots L_0^{-1} \epsilon_{a_s},$$

(4.11)

$$\hat{\mathbb{L}}^* = L_0 \hat{I} + \sum_{s=1}^{\infty} \sum_{a_1, \ldots, a_s=1}^P (-1)^{s+1} \hat{\mathbb{A}}_{a_1 \ldots a_s} \epsilon_{a_1} L_0^{-1} \epsilon_{a_2} L_0^{-1} \ldots L_0^{-1} \epsilon_{a_s},$$

(4.12)

for $\hat{\mathbb{L}}(\vec{r})$ and $\hat{\mathbb{L}}^*$ in powers of the $\epsilon_a$'s with coefficients

$$\hat{\mathbb{A}}_{a_1 \ldots a_s}(\vec{r}) = \int_{\Omega} d\vec{r}' \hat{\mathbb{K}}_{a_1 \ldots a_s}(\vec{r}, \vec{r}')$$

$$= \int_{\Omega} d\vec{r}' [ (I - \hat{\Gamma}_1) \hat{\Lambda}_{a_1} \hat{\Gamma}_1 \hat{\Lambda}_{a_2} \hat{\Gamma}_1 \ldots \hat{\Gamma}_1 \hat{\Lambda}_{a_s}] (\vec{r}, \vec{r}'),$$

(4.13)

$$\hat{\alpha}_{a_1 \ldots a_s} = \int_{\Omega} d\vec{r} \hat{\mathbb{A}}_{a_1 \ldots a_s}(\vec{r})$$

$$= \int_{\Omega} d\vec{r} \int_{\Omega} d\vec{r}' \hat{\mathbb{A}}_{a_1 \ldots a_s}(\vec{r}, \vec{r}')$$

(4.14)

where the prefactor of $(I - \hat{\Gamma}_1)$ has been dropped from the last equation because $\hat{\Gamma}_1$ acting upon any field produces a field with zero integral over $\Omega$: see (2.21).

As a consequence of (2.19), (2.21) and (3.7) the coefficients $\hat{\alpha}_{a_1 \ldots a_s}$ when $s > 1$ satisfy

\[
\sum_{a_1=1}^{P} \hat{\alpha}_{a_1 \ldots a_s} = 0, \tag{4.15}
\]

\[
\sum_{a_s=1}^{P} \hat{\alpha}_{a_1 \ldots a_s} = 0, \tag{4.16}
\]

\[
\sum_{a_1=1}^{P} \hat{\alpha}_{a_1 \ldots a_s} = \hat{\alpha}_{a_1 \ldots a_{s-1} a_{s+1} \ldots a_s}. \tag{4.17}
\]

In the special case $s = 1$ (3.7) implies

\[
\sum_{a=1}^{P} \hat{\alpha}_a = \hat{I}. \tag{4.18}
\]

Due to these identities it suffices, for any choice of reference index $q \in \{1, 2, \ldots, p\}$, to consider the subset of coefficients $\hat{\alpha}_{a_1 \ldots a_s}$, $s = 1, 2, \ldots$ generated as the indices $a_i$ range over the reduced set $\{1, 2, \ldots, q-1, q+1, \ldots, P\}$ skipping the reference index $q$. The remaining coefficients $\hat{\alpha}_{a_1 \ldots a_s}$ where at least one index $a_i = q$ can then be recovered using (4.15)-(4.18). In addition, recall from (2.26) that the operator $\hat{\Gamma}_1$ is self-adjoint (this is also evident from (4.22) below). Also $\hat{\Lambda}_a$ is obviously self-adjoint. So (4.14) implies that the matrix $\hat{\alpha}_{a_1 \ldots a_s}$ is transformed to its transpose under reversal of the ordering of its subscripts:

$$\hat{\alpha}_{a_s a_{s-1} \ldots a_2 a_1} = (\hat{\alpha}_{a_1 a_2 \ldots a_s})^T. \tag{4.19}$$
There are further identities satisfied by the coefficients $\hat{\alpha}_{a_1 \ldots a_s}$. In particular, the first order coefficients satisfy
\[
\text{Tr}(\hat{\alpha}_a) = \text{Tr}(\hat{\alpha}_\beta) = \int_{\Omega} d\vec{r} \text{ Tr}(\hat{\Lambda}_\beta) = m_l f_l,
\]
(4.20)
where $f_l$ denotes the volume fraction occupied by component $l$ and $m_l$ takes values 1, 2 or 3 according to whether the component $l$ has orthorhombic symmetry, uniaxial symmetry, or isotropic symmetry. The last identity in (4.20) follows immediately for orthorhombic components by taking the trace in (3.4) (i.e. $\text{Tr}[\hat{\alpha}_l \hat{\beta}](\vec{r}) = \chi_l(\vec{r})$), and for isotropic components by taking the trace in (3.5) (i.e. $\text{Tr}[\hat{\alpha}_l \hat{\beta}](\vec{r}) = 3 \chi_l(\vec{r})$).

The trace of the second order coefficient $\hat{\alpha}_{ab}$ can also be easily evaluated when the components are isotropic. To see this let us, for simplicity, suppose that the composite material is periodic with periodicity $h$ much smaller than the dimensions of $\Omega$. The action of $\hat{\Gamma}_1$ on any $h$-periodic vector field $\vec{u}(\vec{r})$ is local in Fourier space and produces a vector field $\vec{v}(\vec{r})$ given by
\[
\vec{v}(\vec{r}) = \hat{\Gamma}_1(\vec{r}) \vec{u}(\vec{r}),
\]
(4.21)
in which $\vec{u}(\vec{k})$ denotes the Fourier component of $\vec{u}(\vec{r})$ and where the matrix $\hat{\Gamma}_1(\vec{k})$ has elements
\[
\{\Gamma_1\}_{ij}(\vec{k}) = k_i k_j / |\vec{k}|^2 \quad \vec{k} \neq 0,

= 0 \quad \vec{k} = 0.
\]
(4.22)
Clearly (4.22) implies
\[
\text{Tr}(\hat{\Gamma}_1(\vec{k})) = 1 \quad \vec{k} \neq 0,

= 0 \quad \vec{k} = 0,
\]
(4.23)
and it follows that the operator
\[
\Gamma(\vec{r}, \vec{r}') \equiv \text{Tr}(\hat{\Gamma}_1(\vec{r}, \vec{r}'))
\]
(4.24)
acts on any $h$-periodic scalar field $u(\vec{r})$ to produce the scalar field
\[
v(\vec{r}) = \int_{\Omega} d\vec{r}' \Gamma(\vec{r}, \vec{r}') u(\vec{r}') = u(\vec{r}) - \int_{\Omega} d\vec{r}' u(\vec{r}').
\]
(4.25)
When the components are isotropic $\hat{\Lambda}_a(\vec{r}) = \Lambda_a(\vec{r}) \hat{I}$ and we have
\[
\text{Tr}(\hat{\alpha}_{ab}) = \int_{\Omega} d\vec{r} \int d\vec{r}' \{\Lambda_a \Gamma \Lambda_b\}(\vec{r}, \vec{r}')

= \int_{\Omega} d\vec{r} \Lambda_a(\vec{r}) \Lambda_b(\vec{r}) - \int_{\Omega} d\vec{r} \Lambda_a(\vec{r}) \int_{\Omega} d\vec{r}' \Lambda_b(\vec{r}')

= \delta_{ab} f_a - f_a f_b,
\]
(4.26)
where again $f_a$ and $f_b$ are the volume fractions of the components $a$ and $b$.

In two-dimensional composites (4.26) is a simple corollary of one of an infinite set of identities satisfied by the coefficients $\hat{\alpha}_{a_1 \ldots a_s}$. These follow from the simple duality observation (see, for example, Keller (1964), Dykhne (1970) and Mendelson (1975)) that a $90^\circ$ rotation, $\hat{R}_\bot$ acting on a curl-free field produces a divergence-free field and vice versa. Equivalently, from (4.22) we see immediately that
\[
\hat{R}_\bot \hat{\Gamma}_1(\hat{R}_\bot)^T = I - \hat{\Gamma}_1 - \hat{\Gamma}_0,
\]
(4.27)
When only one field is present, i.e. \( n = 1 \), then the knowledge of the series expansion of \( \hat{L}^s \) in powers of the \( \varepsilon_a \) up to a given order \( s \) is insufficient to determine the coefficients \( \hat{\alpha}^s_{a_1 \ldots a_s} \) when \( p \geq 3 \) and \( s \geq 3 \). For example, consider the problem of electrical conductivity,

\[
\nabla \cdot J(\vec{r}) = 0, \quad \nabla \times E(\vec{r}) = 0, \quad J(\vec{r}) = \sigma(\vec{r})E(\vec{r}), \quad \sigma(\vec{r}) = \sum_{a=1}^{p} \sigma_a \Lambda_a,
\]

in a nearly homogeneous, nearly isotropic material with small values of the conductivity differences

\[
\varepsilon_a = \sigma_a - \sigma_o. \tag{4.35}
\]

Since the scalar quantities \( \sigma_o \) and \( \varepsilon_a \) commute, \( 4.12 \) reduces to the well-known series expansion for the effective conductivity

\[
\hat{\sigma}^s = \sigma_o \hat{I} + \sum_{s=1}^{\infty} \sum_{a_1, \ldots, a_s = 1}^{p} (-1)^{s+1} \hat{\beta}^s_{a_1 \ldots a_s} \varepsilon_{a_1} \varepsilon_{a_2} \ldots \varepsilon_{a_s} / (\sigma_o)^{s-1}, \tag{4.36}
\]

where \( \sigma_o \) is the conductivity of the matrix and \( \varepsilon_a \) are the conductivity differences of the inclusions. The coefficients \( \hat{\alpha}^s_{a_1 \ldots a_s} \) are determined by the series expansions of the effective conductivity tensor \( \hat{\sigma}^s \) up to a given order \( s \).
with coefficients
\[ \hat{\beta}_{a_1...a_s} = [\hat{\alpha}_{a_1...a_s}]_{\text{sym}} \equiv \frac{1}{s!} \sum_{\text{permutations}} \hat{\alpha}_{p(a_1...a_s)}, \] (4.37)

where the brackets \([ \ ]_{\text{sym}}\) denote a symmetrization over all \(s!\) permutations \(p(a_1...a_s)\) of the field indices \(a_1...a_s\), excluding the space indices. In view of (4.19) we have, for example,
\[ \hat{\beta}_{a_1} = \hat{\alpha}_{a_1}, \quad \hat{\beta}_{a_1a_2} = \frac{1}{2}[\hat{\alpha}_{a_1a_2} + (\hat{\alpha}_{a_1a_2})^T], \]
\[ \hat{\beta}_{a_1a_2a_3} = \frac{1}{6}[\hat{\alpha}_{a_1a_2a_3} + \hat{\alpha}_{a_2a_3a_1} + \hat{\alpha}_{a_3a_1a_2} + (\hat{\alpha}_{a_1a_2a_3} + \hat{\alpha}_{a_2a_3a_1} + \hat{\alpha}_{a_3a_1a_2})^T]. \] (4.38)

If the coefficients \(\hat{\beta}_{a_1...a_j}\) are known for all \(j \leq m\) then it is clearly impossible to recover all the coefficients \(\hat{\alpha}_{a_1...a_s}\) for \(s \leq m\): one can only recover the linear combinations given by (4.37). However this does not eliminate the possibility that the coefficients \(\hat{\alpha}_{a_1...a_s}\) could be recovered from knowledge of the entire infinite set of coefficients \(\hat{\beta}_{a_1...a_j}\). As we will see in the Section 7 the value \(\hat{\alpha}_{a_1...a_s}\) can take is nonlinearly correlated with the coefficients \(\hat{\beta}_{a_1...a_j}\) with \(j \leq m\) through a set of matrix inequalities and it is conceivable that these matrix inequalities are sufficiently stringent to uniquely determine a given coefficient \(\hat{\alpha}_{a_1...a_s}\) as \(m\) tends to infinity.

5 The weights and normalization matrices and a stratification of the Hilbert space

Suppose the coefficients \(\hat{A}_{a_1...a_s}(\vec{r})\) of the microscopic response tensor \(\hat{\mathbf{C}}(\vec{r})\) are known as functions of \(\vec{r}\), for all \(s\) up to a given order \(m\), and for all combinations of indices \(a_i\) taken from the set \(\{1, 2, ..., p\}\). In light of (4.13) one might think that this information would only be sufficient to determine the coefficients \(\hat{\alpha}_{a_1...a_s}\) for \(s \leq m\). However this does not take into account the relations
\[ \int d\vec{r} [\hat{A}_{a_1a_2...a_s}(\vec{r})]^T \Lambda_{a_1a_2...a_s}(\vec{r}) = \delta_{a_1a_2...a_s}, \] (5.1)

implied by (4.13), (2.19) and (3.6). These relations, which hold for all \(i \in \{1, 2, ..., s-1\}\), allow the coefficients \(\hat{\alpha}_{a_1...a_s}\) to be determined for \(s \leq 2m\) from knowledge of the functions \(\hat{A}_{a_1...a_s}(\vec{r})\) for all \(s \leq m\).

Now note that (4.14) and (5.1) imply inequalities such as the positive semidefiniteness of the tensors \(\hat{\alpha}_{aa}\) and \(\hat{\alpha}_a - \hat{\alpha}_{aa}\), \(a = 1, 2, ..., p\). The question of what other inequalities apply to the coefficients \(\hat{\alpha}_{a_1...a_s}\) has been analyzed in depth by Milton (1987a, 1987b). Briefly, and as proved later section 7, the set of coefficients \(\hat{\alpha}_{a_1...a_s}\) for \(s \leq 2m\) derive from, and in turn uniquely determine, a set of normalization matrices \(\hat{N}^i\), \(j = 1, 2, ..., m\), and weight matrices \(\hat{W}^i\), \(a = 1, 2, ..., p\), \(j = 0, 1, 2, ..., m-1\) that are real and symmetric and satisfy
\[ \hat{N}^i \geq 0, \quad \hat{W}^i \geq 0, \quad \sum_{a=1}^p \hat{W}^i_a = I^j, \] (5.2)
where \( \hat{1}^j \) denotes the \( k \)-dimensional identity matrix, where in a space of 3 dimensions, \( k = 3(p-1)^j \). These matrices have elements \( N_{\tau, \mu}^j, W_{\alpha, \tau, \mu}^j \) and

\[
I_{\tau, \mu}^j = \delta_{\tau, \mu},
\] (5.3)

labeled by strings \( \tau = a_1a_2...a_j \alpha \) and \( \mu = b_1b_2...b_j \beta \) of integers \( a_i \) or \( b_i, i = 1, 2, ... j \) chosen from the set \( \{1, 2, ..., q − 1, q + 1, 2 \} \) (skipping the reference index \( q \)) terminated by a single space index \( \alpha \) or \( \beta \) chosen from the set \( \{1, 2, 3\} \). Thus each matrix has dimension \( 3(p-1)^j \) dependent on \( j \), for \( p > 2 \).

Conversely, if a set of \( \hat{\alpha}^a_{a_1...a_s} \) derive from any sequence of \( 3(p-1)^j \)-dimensional symmetric real matrices \( \hat{N}^j, j = 1, 2, ... \) and \( \hat{W}^1_a, a = 1, 2, ... p, j = 0, 1, 2, ... \) satisfying (5.2) then there always exists a set of commuting projection operators, \( \hat{\Lambda}_a, a = 1, 2, ... p, \) satisfying (3.6) and (5.4), and another noncommuting projection operator \( \hat{\Gamma}_1 \), satisfying (2.19) such that \( \hat{\alpha}^a_{a_1...a_s} \) is given by (1.14): we will see in Section 7 that, with a suitable choice of basis, the operators \( \hat{\alpha}^a_{a_1...a_s} \) only depend on the weight matrices, while \( \hat{\Gamma}_1 \) in this representation only depends on the normalization matrices. However not every sequence of normalization and weight matrices corresponds to a composite: there are additional subtle restrictions on the operators \( \hat{\alpha}^a_{a_1...a_s} \) and \( \hat{\Gamma}_1 \) in a composite which lead to nontrivial restrictions on the coefficients \( \hat{\alpha}^a_{a_1...a_s} \). In particular, as noticed by Zhikov, Kozlov, and Oleinik (1994), when all the components are isotropic a theorem of Meyers (1963) implies that, in the limit as the volume fraction \( f_a \) of component \( a \) tends to zero, \( \hat{L}^* \) cannot depend on \( \hat{L}_a \) unless of course \( \hat{L}_a \) has infinite or zero eigenvalues. In other words there exist inequalities which force any coefficient \( \hat{\alpha}^a_{a_1...a_s} \), with \( a_i = a \) for some \( i \in \{1, 2, ..., s\} \), to approach zero as \( f_a = \text{Tr}(\hat{\alpha}_a) \) tends to zero.

It remains to link the expansion coefficients with the weight and normalization matrices and to derive suitable representations for the operators \( \hat{\alpha}^a_{a_1...a_s} \) and \( \hat{\Gamma}_1 \). In the rest of the Chapter, lower-case greek letters, other than \( \alpha \) or \( \beta \) will always be used to denote strings of indices, where each index except the last is an element of the set \( \{1, 2, ..., q − 1, q + 1, 2 \} \) and where the final space index takes values from the set \( \{1, 2, 3\} \). The length \( j \) of a string will refer to the number of indices in the string excluding the final space index. Also we use commas to separate strings of indices that label the elements of a matrix. Finally, a \( \leftrightarrow \) above a character accompanied by a superscript \( j \) will indicate a \( 3(p-1)^j \) dimensional matrix in the string indices, with strings of length \( j \).

First consider the sequence of fields obtained in the following fashion. We begin with a set of three or two uniform fields \( \vec{x}_\alpha, (\alpha = 1, 2, 3) \) each aligned with its corresponding coordinate axis. [The notation is somewhat bad as \( \vec{x}_\alpha \) should not be confused with a variable or spatial coordinate, but it follows the notation given in appendix 1 of Milton (1987a).] Then we set

\[
\vec{p}_{a_1a_2...a_k\alpha}(\vec{r}) = \hat{\alpha}^a_{a_1} \hat{\Gamma}_1 \hat{\alpha}^a_{a_2} \hat{\Gamma}_1 ... \hat{\alpha}^a_{a_k} \hat{\Gamma}_1 \hat{x}_{\alpha},
\] (5.4)

\[
\vec{e}_{a_1a_2...a_k\alpha}(\vec{r}) = \hat{\alpha}^a_{a_1} \hat{\Gamma}_1 \hat{\alpha}^a_{a_2} \hat{\Gamma}_1 ... \hat{\alpha}^a_{a_k} \hat{\Gamma}_1 \hat{x}_{\alpha}.
\] (5.5)

Note that the response coefficients \( \hat{\alpha}^a_{a_1...a_s}(\vec{r}) \) derive from these fields: from (4.13) we have

\[
\hat{\alpha}^a_{a_1...a_s}(\vec{r}) \vec{x}_{\alpha} = \vec{p}_{a_1...a_s\alpha}(\vec{r}) - \vec{e}_{a_1...a_s\alpha}(\vec{r}).
\] (5.6)

Introducing the standard inner product,

\[
(\vec{u}, \vec{v}) = \int_{\Omega} d\vec{r} \ \overline{\vec{u}(\vec{r})} \cdot \vec{v}(\vec{r}),
\] (5.7)
between any two real fields \( \bar{u}(\bar{r}) \) and \( \bar{v}(\bar{r}) \), where the overline denotes complex conjugation, it is clear (see also (5.1)) that the inner product between any pair of the above fields can be written in terms of the elements of the coefficient matrix \( \bar{a}_{\alpha_1...\alpha_s} \): we have

\[
(\bar{e}_{\tau}, \bar{e}_{\eta}) = \alpha_{\tau\eta}, 
\]

\[
(\bar{e}_{\tau}, \bar{p}_{\eta}) = (\bar{p}_{\tau}, \bar{e}_{\eta}) = \alpha_{\tau\eta}, 
\]

\[
(\bar{p}_{a\tau}, \bar{p}_{a\eta}) = \delta_{ab} \alpha_{\tau\eta},
\]

where \( \tau \) and \( \eta \) represent strings of indices of lengths \( j \) and \( k \) respectively, and \( \bar{r} \) is obtained from \( r \) by reversing the sequence of indices in the string.

The space spanned by these fields has a natural stratification into a sequence of orthogonal subspaces \( \mathcal{X}^0, \mathcal{Y}^1, \mathcal{X}^1, \mathcal{Y}^2, \mathcal{X}^2, ... \). The subspace \( \mathcal{X}^0 \) is defined as the subspace spanned by the uniform fields \( \bar{x}_\alpha \), \( \alpha = 1, 2, 3 \). Let \( \mathcal{F}^j \) denote the subspace spanned by the fields \( \bar{x}_\alpha, \bar{p}_\eta(\bar{r}) \) and \( \bar{e}_\eta(\bar{r}) \) as \( \eta \) ranges over all strings of length \( j \). Also let \( \mathcal{G}^j \) denote the closure of \( \mathcal{F}^{j-1} \) under the action of the set of operators \( \tilde{\Lambda}_a \ a = 1, 2, ..., p \): this is the space spanned by \( \mathcal{F}^{j-1} \) and fields \( \bar{p}_\tau \) as \( \tau \) ranges over strings of length \( j \). Note that \( \mathcal{F}^j \) in turn is the closure of \( \mathcal{G}^j \) under the action of \( \tilde{\Gamma}_1 \). These subspaces satisfy the inclusion relations

\[
\mathcal{X}^0 = \mathcal{F}^0 \subset \mathcal{G}^1 \subset \mathcal{F}^1 \subset \mathcal{G}^2 \subset \mathcal{F}^2 \subset \mathcal{G}^3 \ldots .
\]

Accordingly we define \( \mathcal{Y}^j, j = 1, 2, ... \) as the subspace of \( \mathcal{G}^j \) which is the orthogonal complement of \( \mathcal{F}^{j-1} \), and \( \mathcal{X}^j, j = 1, 2, ... \) as the subspace of \( \mathcal{F}^j \) which is the orthogonal complement of \( \mathcal{G}^j \).

The weights and normalization matrices are obtained through the introduction of an orthonormal basis set of fields, comprised of fields \( \bar{x}_\eta(\bar{r}) \), denoted as type \( x \), and fields \( \bar{y}_\eta(\bar{r}) \), denoted as type \( y \), generated by a special version of Gram-Schmidt orthogonalization applied to the sequence of fields \( \bar{p}_\tau(\bar{r}) \) and \( \bar{e}_\tau(\bar{r}) \). These basis fields \( \bar{x}_\eta(\bar{r}) \) and \( \bar{y}_\eta(\bar{r}) \) will be called fields of order \( j \) if the string \( \eta \) has length \( j \). Any linear combination of type \( x \) (or type \( y \)) basis fields of order \( j \) will also be called a type \( x \) (or type \( y \)) field of order \( j \) and we will establish that these type \( x \) (or type \( y \)) fields of order \( j \) are precisely the fields in the subspace \( \mathcal{X}^j \) (or \( \mathcal{Y}^j \)).

6 Construction of the basis fields and weights and normalization factors

Those readers not interested in the details of the construction of the basis fields and weight and normalization matrices can skip to Section 9. We follow the construction procedure outlined in Appendix 1 of [Milton (1987a)]. Recall that the uniform fields \( \bar{x}_\alpha \) are already defined. Let us therefore suppose, for some \( j \geq 1 \), that all type \( x \) basis fields of order \( j - 1 \) have been introduced. The weight matrices \( W_{a,\omega,\rho}^{j-1} \) are then defined via

\[
W_{a,\omega,\rho}^{j-1} \equiv \left( \bar{x}_\omega, \tilde{\Lambda}_a \bar{x}_\rho \right),
\]

where \( \omega \) and \( \rho \) are strings of length \( j - 1 \). Next we introduce the first set of auxiliary fields

\[
\bar{a}_{\alpha \omega}(\bar{r}) \equiv \tilde{\Lambda}_a(\bar{r}) \bar{x}_\omega(\bar{r}) - \sum_\zeta W_{a,\omega,\zeta}^{j-1} \bar{x}_\zeta(\bar{r}),
\]

which are defined in this way to ensure orthogonality to the previous set of type \( x \) fields of order \( j - 1 \). Also from (3.7) it is evident that

\[
\sum_{a=1}^p \bar{a}_{\alpha \omega}(\bar{r}) = 0,
\]
and consequently it suffices to consider the subset of fields \( \bar{a}_{a\omega}(\vec{r}) \) as the index \( a \) ranges over the reduced set \( \{1, 2, \ldots, q - 1, q + 1, \ldots p\} \). The inner products between the fields in this subset are given by

\[
(\bar{a}_{a\omega}, \bar{a}_{b\rho}) = Y^j_{a\omega, b\rho},
\]

where

\[
Y^j_{a\omega, b\rho} = \delta_{ab} W^j_{a,\omega, \rho} - \sum_\zeta W^j_{a,\omega, \zeta} W^j_{b,\zeta, \rho},
\]

and the indices \( a \) and \( b \) belong to the reduced set (as does any other index in the strings \( \omega \) and \( \rho \) apart from the terminating index). We normalize these fields to obtain the desired family of type \( y \) basis fields of order \( j \),

\[
\bar{y}_{b\rho} = \sum_{a \neq q} \sum_\omega C^j_{b\rho, a\omega} \bar{a}_{a\omega}
\]

\[
= \sum_{a \neq q} \sum_\omega C^j_{b\rho, a\omega} (\bar{\Lambda}^j_a \bar{x}_{\omega} - \sum_\zeta W^j_{a,\omega, \zeta} \bar{x}_{\zeta}),
\]

where

\[
\bar{\Lambda}^j_a \equiv (\bar{\Lambda}^j)^{-1/2}.
\]

Similarly, starting from these fields, let us introduce the commuting pair of matrices

\[
U^j_{\tau, \phi} = (\bar{y}_{\tau}, \Gamma_1 \bar{y}_{\phi}),
\]

\[
V^j_{\tau, \phi} = (\bar{y}_{\tau}, (I - \Gamma_1) \bar{y}_{\phi}) = \delta_{\tau, \phi} - U^j_{\tau, \phi},
\]

where the string indices \( \tau \) and \( \phi \) are now of length \( j \). In terms of these matrices the normalization matrix is defined via

\[
\hat{N}^j \equiv (\hat{U}^j)^{-1} - \hat{V}^j,
\]

implying

\[
\hat{U}^j = (\hat{I}^j + \hat{N}^j)^{-1}, \quad \hat{V}^j = (\hat{I}^j + (\hat{N}^j)^{-1})^{-1}.
\]

Next we generate the second set of auxiliary fields

\[
\bar{b}_{\tau}(\vec{r}) \equiv \int_{\Omega} \bar{y}_{\tau}(\vec{r}, \vec{r}') \Gamma_1(\vec{r}, \vec{r}') \bar{y}_{\tau}(\vec{r}') - \sum_\nu U^j_{\tau, \nu} \bar{y}_{\nu}(\vec{r}),
\]

which are orthogonal to the fields \( \bar{y}_{\phi} \), and have inner products

\[
(\bar{b}_{\tau}, \bar{b}_{\phi}) = \sum_\nu U^j_{\tau, \nu} V^j_{\nu, \phi}.
\]

Normalizing these fields then produces the next orthonormal set of type \( x \) basis fields of order \( j \):

\[
\bar{x}_{\phi} \equiv \sum_\tau D^j_{\phi, \tau} \bar{b}_{\tau} = \sum_\tau D^j_{\phi, \tau} (\hat{\Gamma}_1 \bar{y}_{\tau} - \sum_\nu U^j_{\tau, \nu} \bar{y}_{\nu}),
\]

where

\[
\hat{D}^j \equiv (\hat{U}^j \hat{V}^j)^{-1/2} = (\hat{N}^j)^{1/2} + (\hat{N}^j)^{-1/2}.
\]

By induction this completes the definition of the basis fields, and weight and normalization matrices.
From the definitions (6.1), (6.5), (6.8) and (6.9) it is clear that the matrices $\hat{W}^{-1}_j$, $\hat{Y}_j^j$, $\hat{U}_j^j$ and $\hat{V}_j^j$ are positive semidefinite. Furthermore from (6.11) and from the orthonormality of the sets of fields, $\vec{x}_\omega$ and $\vec{y}_\tau$, it follows that the weights and normalization matrices satisfy (5.2). We avoid considering the rather special limiting case where the matrices $\hat{W}^{-1}_j$, $\hat{U}_j^j$ and $\hat{V}_j^j$ have zero eigenvalues. In this event the matrices $\hat{Y}_j^j$ and $\hat{U}_j^j\hat{V}_j^j$ become singular and technical difficulties arise in the above construction procedure because the inverses needed in (6.7) and (6.15) do not exist.

The set of normalization and weight matrices obtained in this way clearly depend on the choice of reference component $q$. However the subspace spanned by type $x$ (or type $y$) fields of order $j$ remains invariant: it is only the basis within each subspace that changes when the choice of reference component is changed. Consequently the eigenvalues of the weight and normalization matrices do not depend on the choice of reference media.

Observe from (6.6) and (6.14) that for $a \neq q$

\[
\hat{\Lambda}_a^{\hat{\omega}}\vec{x}_\omega = \sum_\zeta W^{-1}_{a,\omega,\zeta}\vec{x}_\zeta + \sum_{b \neq q} \sum_\rho M^j_{a\omega,\rho\rho}\vec{y}_\rho, \quad (6.16)
\]

\[
\hat{\Gamma}_1^{\hat{\nu}}\vec{y}_\nu = \sum_\nu U^j_{\tau,\nu}\vec{y}_\nu + \sum_\phi X^j_{\tau,\phi}\vec{x}_\phi, \quad (6.17)
\]

where

\[
\hat{X}^j \equiv \left(\hat{U}^j\hat{V}^j\right)^{1/2} = \left\{\left(\hat{N}^j\right)^{1/2} + \left(\hat{N}^j\right)^{-1/2}\right\}^{-1}. \quad (6.18)
\]

\[
\hat{M}^j \equiv \left(\hat{Y}^j\right)^{1/2} = \left(\hat{C}^j\right)^{-1}, \quad (6.19)
\]

and $\hat{Y}^j$ in turn is given by (6.5).

Applying $\hat{\Lambda}_c$, with $c \neq q$ to both sides of this first equation and $\hat{\Gamma}_1$ to both sides of the second equation gives

\[
\sum_{b \neq q} \sum_\rho M^j_{a\omega,\rho\rho}\hat{\Lambda}_c^{\hat{\rho}}\vec{y}_\rho = \sum_\zeta \left(\delta_{ac}\delta_{\omega\zeta} - W^{-1}_{a,\omega,\zeta}\right)\hat{\Lambda}_c^{\hat{\omega}}\vec{x}_\zeta, \quad (6.20)
\]

\[
\sum_\phi X^j_{\tau,\phi}\hat{\Gamma}_1^{\hat{\nu}}\vec{y}_\nu = \sum_\nu V^j_{\tau,\nu}\hat{\Gamma}_1^{\hat{\nu}}\vec{y}_\nu. \quad (6.21)
\]

Substituting (6.16) and (6.17) back into these expressions produces after some algebraic manipulation,

\[
\hat{\Lambda}_c^{\hat{\omega}}\vec{y}_\omega = \sum_{a \neq q} \sum_\zeta Q^j_{\epsilon,\rho,ac}\vec{x}_\zeta + \sum_\zeta M^j_{\rho,\rho\rho}\vec{x}_\zeta, \quad (6.22)
\]

\[
\hat{\Gamma}_1^{\hat{\nu}}\vec{x}_\nu = \sum_\phi V^j_{\nu,\phi}\vec{x}_\phi + \sum_\phi X^j_{\nu,\phi}\vec{y}_\phi, \quad (6.23)
\]

where $\hat{Q}^j_{\epsilon}$ is the matrix,

\[
\hat{Q}^j_{\epsilon} \equiv \hat{M}^j_{\epsilon}\left(\hat{W}^{-1}\right)\left(\hat{M}^j_{\epsilon}\right)^T, \quad (6.24)
\]

and $\hat{M}^j_{\epsilon}$, with transpose $\left(\hat{M}^j_{\epsilon}\right)^T$, is the rectangular submatrix of the square matrix $\hat{M}^j$ defined in (6.19) with elements $M^j_{\alpha\tau,\lambda}$ labeled by the strings $\tau$ and $\lambda$.

So $\hat{\Lambda}_c$ acting upon any basis field produces a linear combination of two fields: one field of the same order and type as the basis field and the other field of adjacent order and opposite
type. By contrast $\Gamma_1$ acting on any basis field produces a field of the same order but mixed type.

By construction the basis fields of a given order form an orthonormal set. To establish the orthonormality of the entire basis set we still need to show that the basis fields of order $j$ are orthogonal to the subspace spanned by the fields of order at most $j-1$. Note that this subspace can also be identified with the subspace $\mathcal{F}^{j-1}$ spanned by the fields $x_\alpha, \vec{p}_\eta(\vec{r})$, and $\vec{e}_\eta(\vec{r})$ as $\eta$ ranges over strings of length $k \leq j - 1$. We argue by induction and begin by assuming that the collection of fields $\vec{x}_\eta$ and $\vec{y}_\eta$ of order at most $j-1$ forms an orthonormal basis of $\mathcal{F}^{j-1}$: this is clearly true when $j=1$ because then $\mathcal{F}^0$ is the three dimensional space spanned by the fields $\vec{x}_\alpha$. In particular the assumption implies that within $\mathcal{F}^{j-1}$ basis fields of different types or different orders are orthogonal. Since $\Lambda_a$ is self-adjoint (6.2) implies that

$$\langle \vec{a}_\omega, \vec{x}_{\eta} \rangle = \langle \vec{x}_{\omega}, \Lambda_a \vec{x}_{\eta} \rangle, \quad \langle \vec{a}_\omega, \vec{y}_{\eta} \rangle = \langle \vec{x}_{\omega}, \Lambda_a \vec{y}_{\eta} \rangle,$$

(6.25)

where the string $\omega$ has length $j-1$. The choice of auxiliary fields guarantees that the first inner product is zero when the length $k$ of the string $\eta$ equals $j-1$. It is also zero when $k < j - 1$ because then (6.16) implies $\Lambda_a \vec{x}_{\eta} \in \mathcal{G}^{j-1}$ where $\mathcal{G}^{j-1}$ can now be identified with the space spanned by fields in $\mathcal{F}^{j-2}$ and type $y$ fields of order $j-1$. Similarly the second inner product is zero because (6.22) implies $\Lambda_a \vec{y}_{\eta} \in \mathcal{G}^{j-1}$. Since these inner products are zero we conclude that the auxiliary fields $\vec{a}_\omega$ are orthogonal to $\mathcal{F}^{j-1}$. The type $y$ fields of order $j$ are linear combinations of these auxiliary fields and so must also be orthogonal to the space $\mathcal{F}^{j-1}$.

Analogous considerations show that the inner products

$$\langle \vec{b}_\tau, \vec{x}_{\eta} \rangle = \langle \vec{y}_{\tau}, \Gamma_1 \vec{x}_{\eta} \rangle, \quad \langle \vec{b}_\tau, \vec{y}_{\eta} \rangle = \langle \vec{y}_{\tau}, \Gamma_1 \vec{y}_{\eta} \rangle,$$

(6.26)

implied by (6.12) are zero when the string $\tau$ has length $j$. We deduce that the type $x$ fields of order $j$ are also orthogonal to the space $\mathcal{F}^{j-1}$. This completes the proof of orthonormality of the basis. As a corollary, it follows that $\mathcal{X}^j$ and $\mathcal{Y}^j$ represent respectively the type $x$ fields and type $y$ fields of order $j$.

7 Representation of the projection operators and recovery of weight and normalization matrices from series expansion coefficients

Clearly (6.16) and (6.22) determine the action of $\Lambda_a$ on the basis fields while (6.17) and (6.23) determine the action of $\Gamma_1$. It immediately follows that the projection operators $\Gamma_1$ and $\Lambda_a$ for $a \neq q$ are represented in this basis by the block tridiagonal infinite matrices

$$\Lambda_a = \begin{bmatrix}
\begin{bmatrix}
W_a^{0} & \Lambda_a^{1} & 0 \\
(\Lambda_a^{1})^T & \Lambda_a^{2} & 0 \\
0 & W_a^{1} & \Lambda_a^2
\end{bmatrix}
\end{bmatrix},$$
In this way we obtain expressions, such as

\[ \hat{\Gamma}_1 = \begin{bmatrix}
\alpha & 0 & 0 \\
0 & \hat{U}^1 & \hat{V}_1 \\
0 & \hat{V}_2 & \hat{U}^2 \\
\end{bmatrix} \]  

(7.1)

The blocks in these matrices act upon fields of the order indicated by the block superscript, with the exception of the rectangular blocks \((M_q^j)^T\) which act on fields of order \(j - 1\). The blocks going across a given row act on fields alternating between type \(x\) and type \(y\), beginning with type \(x\). The tridiagonal form of the matrices representing \(\hat{\Gamma}_1\) and \(\hat{\Lambda}_a\) reflects the fact that the procedure for constructing the basis fields is similar to the procedure used in the Lanczos algorithm for tridiagonalization of symmetric matrices (see, for example, Strang 1986). The operator

\[ \hat{\Lambda}_q = I - \sum_{a \neq q} \hat{\Lambda}_a \]  

(7.2)

also can be represented by the matrix in (7.1) with \(a = q\) provided we define \(\hat{M}_q^j\) via

\[ \hat{M}_q^j \equiv - \sum_{a \neq q} \hat{M}_a^j, \]  

(7.3)

and \(Q_q^j\) via (6.24). The matrix representing \(\hat{\Lambda}_a \hat{\Gamma}_1 \hat{\Lambda}_a \hat{\Gamma}_1 \ldots \hat{\Gamma}_1 \hat{\Lambda}_a\) is generated by taking products of the matrices in (7.1). Also for any operator \(\tilde{B}(\vec{r}, \vec{r}')\) with elements \(\tilde{B}_{\alpha\beta}(\vec{r}, \vec{r}')\) we have

\[ \int_{\Omega} d\vec{r} \int_{\Omega} d\vec{r}' \tilde{B}_{\alpha\beta}(\vec{r}, \vec{r}') = (\vec{x}_\alpha, \tilde{\hat{B}} \vec{x}_\beta). \]  

(7.4)

In particular then \(\tilde{\hat{a}}_{a_1 \ldots a_s}\) is the first block which appears in the matrix representing \(\hat{\Lambda}_a \hat{\Gamma}_1 \hat{\Lambda}_a \hat{\Gamma}_1 \ldots \hat{\Gamma}_1 \hat{\Lambda}_a\). In this way we obtain expressions, such as

\[ \tilde{\hat{a}}_{a_1} = \tilde{W}_{a_1}^0, \]  

(7.5)

\[ \tilde{\hat{a}}_{a_1 a_2} = \tilde{M}_{a_1}^1 \tilde{U}^1 (\tilde{M}_{a_2}^1)^T, \]  

(7.6)

\[ \tilde{\hat{a}}_{a_1 a_2 a_3} = \tilde{M}_{a_1}^1 \tilde{U}^1 Q_{a_2}^1 \tilde{U}^1 (\tilde{M}_{a_3}^1)^T + \tilde{M}_{a_1}^1 \tilde{X}^1 \tilde{W}_{a_2}^1 \tilde{X}^1 (\tilde{M}_{a_3}^1)^T, \]  

(7.7)

\[ \tilde{\hat{a}}_{a_1 a_2 a_3 a_4} = \tilde{M}_{a_1}^1 \tilde{U}^1 Q_{a_2}^1 \tilde{U}^1 Q_{a_3}^1 \tilde{U}^1 (\tilde{M}_{a_4}^1)^T + \tilde{M}_{a_1}^1 \tilde{U}^1 Q_{a_2}^1 \tilde{X}^1 \tilde{W}_{a_3}^1 \tilde{X}^1 (\tilde{M}_{a_4}^1)^T + \tilde{M}_{a_1}^1 \tilde{X}^1 \tilde{W}_{a_2}^1 \tilde{X}^1 Q_{a_3}^1 \tilde{U}^1 (\tilde{M}_{a_4}^1)^T + \tilde{M}_{a_1}^1 \tilde{X}^1 \tilde{W}_{a_2}^1 \tilde{X}^1 \tilde{W}_{a_3}^1 \tilde{X}^1 (\tilde{M}_{a_4}^1)^T + \tilde{M}_{a_1}^1 \tilde{X}^1 \tilde{X}^1 \tilde{W}_{a_2}^2 \tilde{X}^2 (\tilde{M}_{a_4}^1)^T, \]  

(7.8)

for the \(\tilde{\hat{a}}_{a_1 \ldots a_s}\) in terms of the normalization and weight matrices. Conversely, if the coefficients \(\tilde{\hat{a}}_{a_1 \ldots a_s}\) are known then (7.5) gives \(\tilde{W}_{a_1}^0\), and (7.6), (7.7), and (7.8) can be solved successively for \(\tilde{U}^1, \tilde{W}_{a_2}^1,\) and \(\tilde{U}^2\). These enter the equations linearly. Prior to solving each one of these
It can be checked through matrix multiplication that the set of matrices $\hat{\Gamma}_1$ and $\hat{\Lambda}_a$ defined via \((7.1)\) are projection operators satisfying \((2.19)\), \((3.6)\), and \((3.7)\) for any choice of normalization and weight matrices satisfying \((5.2)\). Consequently any further restrictions on the set of possible normalization and weight matrices must come from additional information about the operators $\hat{\Gamma}_1$ and $\hat{\Lambda}_a$, such as the identity \((4.27)\) which holds for two-dimensional composites.

Note that we have only shown that the weights and normalization matrices can be recovered from the coefficients $\alpha_{a_1...a_s}$. A separate question, which we do not address, is whether these coefficients can be recovered from the series expansion \((4.12)\) in powers of the elements of the matrices $\epsilon_a$, $a = 1, 2, \ldots, p$. Since the matrix $\epsilon_a L_0^{-1}$ does not generally commute with $\epsilon_b L_0^{-1}$, when $b \neq a$ it seems likely that one should be able to recover the coefficients $\alpha_{a_1...a_s}$ if $p$ was sufficiently large. But without a proof the most we can say is what we said in the introduction: that the series probably contains sufficient information to determine the weight and normalization matrices.

## 8 Simplification for two-dimensional, isotropic composites

It can be checked through matrix multiplication that the set of matrices $\hat{\Gamma}_1$ and $\hat{\Lambda}_a$ defined via \((7.1)\) are projection operators satisfying \((2.19)\), \((3.6)\), and \((3.7)\) for any choice of normalization and weight matrices satisfying \((5.2)\). Consequently any further restrictions on the set of possible normalization and weight matrices must come from additional information about the operators $\hat{\Gamma}_1$ and $\hat{\Lambda}_a$, such as the identity \((4.27)\) which holds for two-dimensional composites.

In particular, if the composite is two-dimensional, statistically isotropic and has isotropic components then \((4.27)\) implies that each normalization matrix is simply the identity matrix. Indeed, the isotropy of the composite implies $\hat{L}^* = \hat{I} L^*$ for all choices of moduli $L_a$ and consequently all the coefficients $\alpha_{a_1...a_s}$ are also proportional to $\hat{I}$. It follows that the weights and normalization matrices are also proportional to $\hat{I}$ in their space indices:

\[
W_{c,a_1...a_s b_1...b_s}^j = w_{c,a_1...a_s b_1...b_s}^j \delta_{\alpha\beta},
\]

\[
N_{a_1...a_s b_1...b_s}^j = n_{a_1...a_s b_1...b_s}^j \delta_{\alpha\beta},
\]

and hence commute with $\hat{R}_\perp$. The isotropy of the components implies $\hat{R}_\perp$ also commutes with the operators $\hat{\Lambda}_a$. We next need to establish that

\[
\hat{R}_\perp \hat{\alpha}_{a_1...a_s} = (-1)^s \sum_{\beta=1}^{2} R_{\alpha\beta}^\perp \hat{\alpha}_{a_1...a_s},
\]

\[
\hat{R}_\perp \hat{\gamma}_{a_1...a_s} = (-1)^{s+1} \sum_{\beta=1}^{2} R_{\alpha\beta}^\perp \hat{\gamma}_{a_1...a_s},
\]
To see this first observe that (4.28) implies that \( \mathcal{F}^j \) and \( \mathcal{G}^j \) are each closed under the action of \( \mathcal{R}_{\perp}^j \), and as a consequence so are the spaces \( \mathcal{X}^j \) and \( \mathcal{Y}^j \). Now we proceed by supposing there exists an \( j \) such that (8.2) holds true for all \( s \leq j - 1 \) and for all permutations of indices: this is clearly true when \( j = 0 \). Now for any strings \( \rho \) and \( \phi \) of length \( j - 1 \geq 0 \), (6.6) and (6.14) imply

\[
\vec{y}_\rho \left[ \sum_{a \neq q} \omega \right] (\Lambda_a \vec{x}_\omega) \in \mathcal{F}^{j-1},
\]

where \( \omega \) has length \( j - 1 \). By our supposition we can use to (8.2) to compute the action of \( \mathcal{R}_{\perp} \) on \( \vec{x}_\omega \). Applying \( \mathcal{R}_{\perp} \) to (8.4) and using (8.1) and (4.28) brings one to the conclusion that

\[
\mathcal{R}_{\perp} \vec{y}_a \cdots a_j \alpha + (-1)^j \sum_{\beta=1}^2 R_{\alpha\beta} \vec{y}_a \cdots a_j \beta \in \mathcal{F}^{j-1},
\]

for all combinations of indices. But \( \mathcal{Y}^j \) is closed under the action of \( \mathcal{R}_{\perp} \) and since \( \mathcal{Y}^j \) is orthogonal to \( \mathcal{F}^{j-1} \) we infer that the field in (8.6) is zero, i.e. that (8.3) holds for \( s = m \).

Applying \( \mathcal{R}_{\perp} \) to (8.5) and using a similar argument establishes that (8.2) holds when \( s = m + 1 \). By induction this completes the proof of (8.2) and (8.3). In turn these imply via (4.27) that

\[
\mathcal{R}_{\perp} \vec{y}_\tau, \vec{y}_\phi = (\vec{y}_\tau, (\mathcal{R}_{\perp})^T \vec{y}_\phi) = (\vec{y}_\tau, (I - \Gamma_1)\vec{y}_\phi) = \delta_{\tau\phi} - \mathcal{R}_{\perp} \vec{y}_\phi.
\]

From the definition (6.10) it follows that

\[
\mathcal{N}^j = \mathcal{I}^j,
\]

and consequently the operator \( \mathcal{I}_1 \) is represented by the matrix

\[
\mathcal{I}_1 = \frac{1}{2} \begin{bmatrix}
0 & 0 & 0 \\
0 & \mathcal{I}_1 & 0 \\
0 & 0 & \mathcal{I}_1
\end{bmatrix},
\]

Note also from (8.2) and (8.3) that \( \mathcal{R}_{\perp} \) has the representation,

\[
\mathcal{R}_{\perp} = \begin{bmatrix}
\mathcal{R}_{\perp}^0 & 0 \\
-\mathcal{R}_{\perp}^1 & \mathcal{R}_{\perp}^1 \\
0 & -\mathcal{R}_{\perp}^2
\end{bmatrix},
\]

where \( \mathcal{R}_{\perp}^j \) is the rotation matrix with elements

\[
R_{a_1 \cdots a_j b_1 \cdots b_j} = R_{a_\beta} \prod_{i=1}^s \delta_{a_i b_i},
\]
When \( p = 2 \) and the composite is two-dimensional but possibly anisotropic, the set of all possible sequences of weight and normalization matrices has been completely characterized, and furthermore microgeometries have been identified which correspond to every such sequence. This was accomplished by [Milton (1986b)] for composites of two isotropic phases and by [Clark and Milton (1994)] for a polycrystal built from a single anisotropic crystal. In both cases the microgeometries that can simulate any sequence were found to be sequentially layered laminates. These two-dimensional microstructures can mimic the entire behavior of \( L^* \) as a function of the component moduli while keeping the microstructure fixed.

9 Bounds and methods for bounding the effective tensor

Bounds on the effective tensor \( L^* \) follow directly from the variational principles,

\[
\tilde{E}_0 \cdot L^* \tilde{E}_0 = \min_{\tilde{e}(\bar{r})} \int_{\Omega} d\bar{r} \left( \tilde{E}_0 + \tilde{e}(\bar{r}) \right) \cdot (L(\bar{r})\tilde{E}_0 + \tilde{e}(\bar{r})), \tag{9.1}
\]

\[
\tilde{J}_0 \cdot (L^*)^{-1} \tilde{J}_0 = \min_{\tilde{j}(\bar{r})} \int_{\Omega} d\bar{r} \left( \tilde{J}_0 + \tilde{j}(\bar{r}) \right) \cdot (L(\bar{r})^{-1}(\tilde{J}_0 + \tilde{j}(\bar{r}))), \tag{9.2}
\]

where \( \tilde{E}_0 \) and \( \tilde{J}_0 \) are uniform fields, and the minimization extends over statistically homogeneous or periodic fields \( \tilde{e}(\bar{r}) \) and \( \tilde{j}(\bar{r}) \) satisfying

\[
\nabla \times \tilde{e}(\bar{r}) = 0, \quad \int_{\Omega} d\bar{r} \tilde{e}(\bar{r}) = 0, \tag{9.3}
\]

\[
\nabla \cdot \tilde{j}(\bar{r}) = 0, \quad \int_{\Omega} d\bar{r} \tilde{j}(\bar{r}) = 0. \tag{9.4}
\]

Substitution of the trial fields \( \tilde{e}(\bar{r}) = 0 \) and \( \tilde{j}(\bar{r}) = 0 \) gives the arithmetic and harmonic mean bounds,

\[
\left[ \sum_{a=1}^{p} \frac{\tilde{\alpha}_a}{\tilde{L}_a} \right]^{-1} \leq L^* \leq \sum_{a=1}^{p} \frac{\tilde{\alpha}_a}{\tilde{L}_a}. \tag{9.5}
\]

Better bounds result from a more judicious choice of trial fields. For example, to derive improved upper bounds one can follow the approach of Beran (1965, 1966) and choose a trial field of the form

\[
\tilde{e}(\bar{r}) = \sum_{s=1}^{j} \sum_{a_1=1}^{p} \sum_{a_2=1}^{3} c_{a_1 a_2 ... a_s} \tilde{e}(\bar{r}), \tag{9.6}
\]

where the fields \( \tilde{e}(\bar{r}) \) are given by (5.5), and then minimize (9.1) to find the best choice of the coefficients \( c_{a_1 a_2 ... a_s} \), which are vectors in the field indices. The bound generated by this procedure when expanded in a power series agrees with the terms in the series (4.12) for all \( s \) up to and including \( s = 2j + 1 \), and for this reason is called the Wiener-Beran type upper bound of order \( 2j + 1 \): a bound is said to be of order \( m \) if the series expansion of the bound and the series expansion of \( L^* \) agree for all \( s \) up to and including \( s = m \). An analogous choice of trial field \( \tilde{j}(\bar{r}) \) generates the Wiener-Beran type lower bound of order \( 2j + 1 \) through the variational principle (9.2). Bounds of even order are generated by substituting an appropriate choice of trial polarization field into the Hashin-Shtrikman variational principles (Hashin and Shtrikman 1962), yielding Hashin-Shtrikman type bounds.

These bounds on \( L^* \) are naturally expressed in terms of the normalization and weight matrices. For this purpose it is useful to expand \( L^* \) as a continued fraction rather than as
a power series. A direct extension of the analysis of Milton (1987a, 1987b) gives a continued fraction expansion for the effective tensor

\[ \hat{L}^* = \hat{L}^* \],

(9.7)
generated by setting

\[ \hat{L}_0 = L_0, \]

(9.8)
and eliminating the tensors \( \hat{L}^{*j} \) for \( j \geq 1 \) from the recursion relations

\[
\hat{L}^{*j-1} = \sum_{a=1}^{p} \hat{W}_a \hat{L}_{a} - \sum_{a,b \neq q} \epsilon_a \hat{M}_a \{ \hat{I} \cdot \hat{L}_0 + \sum_{c \neq q} \hat{Q}_c \epsilon_c + (\hat{N}^j)^{1/2} \hat{L}^{*j} (\hat{N}^{*j})^{1/2} \}^{-1} (\hat{M}_b)^T \epsilon_b,
\]

(9.9)
where, in accordance with our previous definitions,

\[
\hat{Q}_c = \hat{M}_c (\hat{W}_c)^{-1} (\hat{M}_c)^T, \quad \hat{M}^j = (\hat{Y}^j)^{1/2}, \quad Y_{\alpha\beta} = \delta_{\alpha\beta} W_{\alpha\beta} - \sum_\zeta W_{\alpha\zeta} W_{\beta\zeta},
\]

(9.10)
and \( \hat{M}_a \), with transpose \( (\hat{M}_a)^T \), is the rectangular submatrix of the square matrix \( \hat{M} \) with elements \( M_{\alpha\tau\lambda} \) labeled by the strings \( \tau \) and \( \lambda \). Note that \( \hat{L}^{*j} \) has elements \( L^{*j}_{\tau\kappa\mu} \) labeled by field indices \( k, m \in \{1, 2, p\} \) and string indices \( \tau = a_1 a_2, a_3, \mu = b_1 b_2 b_3 \) with \( a_i \) and \( b_i \in \{1, 2, ...q - 1, q + 1, ...p\} \), and \( \alpha \) and \( \beta \in \{1, 2, 3\} \). Also note that \( \hat{W}_a, \hat{M}_a \) and \( \hat{N}^j \) act on the string indices, not on the field indices.

There are other equivalent ways of expressing \( \hat{L}^{*j-1} \) in terms of \( \hat{L}^{*j} \) (Milton 1987a). For example (9.9) can be replaced by its dual form

\[
(\hat{L}^{*j-1})^{-1} = \sum_{a=1}^{p} \hat{W}_a (L_a)^{-1} - \sum_{a,b \neq q} \eta_a \hat{M}_a \{ \hat{I} \cdot L_0 - \sum_{c \neq q} \hat{Q}_c \eta_c + (\hat{N}^j)^{-1/2} (\hat{L}^{*j})^{-1} (\hat{N}^{*j})^{-1/2} \}^{-1} (\hat{M}_b)^T \eta_b,
\]

(9.11)
where

\[ \eta_a \equiv (L_a)^{-1} - L_0^{-1}. \]

(9.12)
Eliminating the matrices \( \hat{L}^{*j} \) from this recursion relation generates an alternative continued fraction expansion of \( \hat{L}^* \).

The tensors \( \hat{L}^{*j}, j = 0, 1, 2, ... \) have an interpretation in the context of the solution \( \vec{J}(\vec{r}) \) for any given field \( \vec{E}_0 \in \mathcal{X}^j \) (the space \( \mathcal{X}^j \) now plays the role that was played by the uniform fields) to the equations

\[
\hat{\Gamma}_1 \hat{J} = 0, \quad \hat{J}(\vec{r}) = \hat{L}(\vec{r})(\vec{E}_0(\vec{r}) + \vec{e}(\vec{r})), \quad \hat{\Gamma}_1 \vec{e} = \vec{e},
\]

(9.13)
where \( \hat{\Gamma}_1 \) is the nonlocal operator,

\[ \hat{\Gamma}_1 = \hat{\Gamma}_1 - \hat{\gamma}^j, \]

(9.14)
and $\vec{Y}^j$ (which commutes with $\vec{\Gamma}_1$) is the projection onto the space
\[ \mathcal{E}^j = \{ \vec{u}(\vec{r}) \in \mathcal{X}^j \otimes \mathcal{Y}^j | \vec{\Gamma}_1 \vec{u} = \vec{u} \} \]  
(9.15)
of order $j$ fields which are curl-free and have zero average value. In the representation $\vec{\Gamma}_1 \vec{\Gamma}_1^j$ is obtained from $\vec{\Gamma}_1$ by setting the blocks $\vec{U}^j, \vec{V}^j$ and $\vec{X}^j$ to zero. Note that $\vec{\Gamma}_1$ is a projection and acts upon any field to produce a curl-free field with zero average value. So in particular $\vec{e}(\vec{r})$ (but not $\vec{E}_0(\vec{r})$) is the gradient of a potential.

A simple application of the Lax-Milgram lemma (see, for example, Section 5.8 of [5.8 of Gilbarg and Trudinger 1983]) shows that these equations always have a unique solution for $\vec{J}(\vec{r})$, for any choice of field $\vec{E}_0 \in \mathcal{X}^j$, provided that the set of tensors $\vec{\Lambda}_a$ are positive definite and bounded. Let us define $\vec{\Gamma}_0^j$ as the projection onto the subspace $\mathcal{X}^j$ and $\vec{J}_0$ as the component of the field $\vec{J}(\vec{r})$ which lies in the subspace $\mathcal{X}^j$. Since the relation between $\vec{J}_0$ and $\vec{E}_0$ is linear we can write
\[ \vec{J}_0 = L^{*j} \vec{E}_0. \]  
(9.17)
This linear relation serves to define $L^{*j}$: it is a linear map from the space $\mathcal{X}^j$ to itself. When $j = 0$ these equations reduce to the previous set (2.3), (2.10), and (2.12) and so we can make the identification (9.7) between $L^*$ and $L^{*0}$.

From the matrix representation (7.1) of the operators $\vec{\Lambda}_a$ and $\vec{\Gamma}_1$ it is clear that $\vec{\Lambda}_a$ and $\vec{\Gamma}_1$ do not couple $\vec{E}_0$ with fields in the space $\mathcal{G}^j$. Thus the fields in $\mathcal{G}^j$ play no role in the solutions of the equations (9.13). Consequently we can now eliminate from our basis those fields $\vec{x}_r, \vec{y}_r \in \mathcal{G}^j$. In the remaining reduced basis the operators $\vec{\Lambda}_a$ and $\vec{\Gamma}_1$ have the representation
\[
\vec{\Lambda}_a = \begin{bmatrix}
\vec{W}_a & \vec{M}_a^{j+1} \\
(M_a^{j+1})^T & \vec{Q}_a^{j+1} \\
\vec{U}_a^{j+1} & \vec{M}_a^{j+2} \\
(M_a^{j+2})^T & \vec{Q}_a^{j+2}
\end{bmatrix},
\]
\[ \vec{\Gamma}_1 = \begin{bmatrix}
0 & 0 & 0 \\
\vec{U}_a^{j+1} & \vec{X}_a^{j+1} & 0 \\
0 & \vec{X}_a^{j+1} & \vec{V}_a^{j+1} \\
0 & 0 & \vec{U}_a^{j+2} & \vec{X}_a^{j+2} & 0 \\
& & & & \ddots
\end{bmatrix}.
\]  
(9.18)
The similarity with (7.1) makes it evident that whatever role the sequence $\vec{W}_a^0, \vec{W}_a^1, \vec{W}_a^2, \vec{W}_a^3, \ldots$ of weight and normalization matrices plays in determining $L^*$ is played in an identical way by the sequence $\vec{W}_a^0, \vec{W}_a^1, \vec{W}_a^2, \vec{W}_a^3, \ldots$ in determining $L^{*j}$. This self-similarity is also evident from the continued fraction expansions for $L^*$ and $L^{*j}$ implied by (9.9).
If the entire set of normalization and weight matrices is known then these continued fractions expansions allow the effective tensor $\hat{\mathbf{L}}^*$ to be computed to an arbitrarily high degree of accuracy. For example we could truncate the continued fraction at some stage $m$ by setting

$$\hat{\mathbf{L}}^m = \hat{\mathbf{I}}^m \hat{\mathbf{L}},$$

(9.19)

which is a natural choice, corresponding to replacing the set of weights $\hat{\mathbf{W}}^m_a$ by the weights

$$\hat{\mathbf{W}}^m_q = \hat{\mathbf{I}}^m, \quad \hat{\mathbf{W}}^m_a = 0, \quad \forall a \neq q,$$

(9.20)

consistent with the constraints (5.2). Then the tensor $\hat{\mathbf{L}}^0$ obtained from the recursion relations (9.9) is an $m$-th order rational approximate to $\hat{\mathbf{L}}^*$, and it can be proved that this approximate converges to $\hat{\mathbf{L}}^*$ as $m$ tends to infinity, for any positive definite bounded set of moduli $\mathbf{L}_a, a = 1, \ldots, p$ (Milton 1987b). The approximates also converge when the moduli are complex, provided the tensors $\mathbf{L}_a$ are symmetric and bounded and such that there exists a phase angle $\theta$ for which

$$\text{Re}(e^{i\theta} \mathbf{L}_a) > 0, \quad \forall a,$$

(9.21)

where $\text{Re}(A)$ denotes the real part of the quantity $A$. Such complex moduli have a physical interpretation. When the fields $\vec{J}$ and $\vec{E}$ oscillate sinusoidally in time $t$ with frequency $\omega$ then they can be expressed as the real part of complex fields $\vec{J}_c(\vec{r})$ and $\vec{E}_c(\vec{r})$,

$$\vec{J}(\vec{r}, \omega) = \text{Re}(e^{i\omega t} \vec{J}_c(\vec{r})), \quad \vec{E}(\vec{r}, \omega) = \text{Re}(e^{i\omega t} \vec{E}_c(\vec{r})).$$

(9.22)

Provided the wavelength of this oscillation is sufficiently large compared with the microstructure these complex fields satisfy the quasistatic equations,

$$\vec{\nabla} \cdot \vec{J}_c(\vec{r}) = 0, \quad \vec{\nabla} \times \vec{E}_c(\vec{r}) = 0, \quad \vec{J}_c(\vec{r}) = \hat{\mathbf{L}}(\vec{r}) \vec{E}_c(\vec{r}),$$

(9.23)

with a complex tensor $\hat{\mathbf{L}}(\vec{r})$ given by

$$\hat{\mathbf{L}}(\vec{r}) = \sum_{a=1}^p \hat{\mathbf{A}}_a \mathbf{L}_a,$$

(9.24)

where the moduli $\mathbf{L}_a$ are complex and frequency dependent. The thermodynamic requirement that dissipation of power into entropy be positive ensures that (9.21) holds when $\theta = 0$. Each rational approximate satisfies the properties of covariance and disjunction, discussed in the introduction, and has the additional required analytic property that

$$\text{Re}(e^{i\theta} \hat{\mathbf{L}}^*) > 0,$$

(9.25)

for any set of tensors $\mathbf{L}_a$ satisfying (9.21).

Bounds on $\hat{\mathbf{L}}^*$ follow from elementary bounds on $\hat{\mathbf{L}}^{*j}$. In particular, the inequalities

$$0 \leq \hat{\mathbf{L}}^{*j} \leq \infty \hat{\mathbf{I}}^j,$$

(9.26)

or equivalently the inequalities

$$\left[\sum_{a=1}^p \hat{\mathbf{W}}^{-1}_a (\mathbf{L}_a)^{-1}\right]^{-1} \leq \hat{\mathbf{L}}^{*j-1} \leq \sum_{a=1}^p \hat{\mathbf{W}}^{-1}_a L_a,$$

(9.27)
when substituted in the recursion relations (9.9) or (9.12) produce the Weiner-Beran type bounds on $\hat{\mathbf{L}}^*$ of order $2j - 1$, while the inequalities

$$L^- \mathbf{{i}}^j \leq \hat{\mathbf{L}}^j \leq L^+ \mathbf{{i}}^j,$$

(9.28)

which hold for all tensors $L^-$ and $L^+$ such that

$$L^- \leq L_a \leq L^+, \quad 1 \leq a \leq p,$$

(9.29)

when substituted in (9.9) or (9.12) produce the Hashin-Shtrikman type bounds on $\hat{\mathbf{L}}^*$ of order $2j$. By substitution we mean precisely that an upper bound on $\hat{\mathbf{L}}^*$ is obtained by setting $\hat{\mathbf{L}}^j = \infty \mathbf{{i}}^j$ or $\hat{\mathbf{L}}^j = L^+$ and solving the recursion relations for $\hat{\mathbf{L}}^*0$ and that a lower bound on $\hat{\mathbf{L}}^*$ is obtained by setting $\hat{\mathbf{L}}^j = 0$ or $\hat{\mathbf{L}}^j = L^-$ and solving for $\hat{\mathbf{L}}^*0$.

10 Bounds using the field-equation recursion method

The inequalities (9.27) and (9.28) can be easily derived without reference to variational principles using the field recursion method for bounding effective tensors. This approach utilizes the recursive structure of the equations (9.9) and the inequalities (5.2) on the normalization and weight matrices. The first step in the method is to conjecture a set of restrictions that might apply to $\hat{\mathbf{L}}^j$ irrespective of what values the weights and normalization matrices take, subject only to the constraints (5.2)-or perhaps additional constraints if these are known. This conjecture need not be very restrictive, and could be guided by the form of the recursion relations (9.9). For example let us conjecture that $\hat{\mathbf{L}}^j$ is positive semidefinite. The next step is to first check that the tensor $\hat{\mathbf{L}}^*m$ given by (9.19) satisfies the conjecture, and indeed it does. Then the remaining task is to assume the conjecture is true for some $j$ and show this implies $\hat{\mathbf{L}}^j-1$ also satisfies the conjecture, for any choice of the weight matrices $\hat{\mathbf{W}}^j-1$ and normalization matrices $\hat{\mathbf{N}}^j$ satisfying (5.2); it obviously does since from the recursion relations (9.9) and (9.11) it follows that (9.26) implies (9.27) which in turn implies $\hat{\mathbf{L}}^j-1$ is positive semidefinite. By induction any rational approximate for $\hat{\mathbf{L}}^j$ generated by choosing $m > j$ and making the substitution (9.19) satisfies the conjecture, and since these approximates converge to $\hat{\mathbf{L}}^j$ as $m$ tends to infinity, we conclude that $\hat{\mathbf{L}}^j$ itself must be positive semidefinite. The conjecture is proved and it clearly implies both (9.27) and (9.28). The recursion method has the advantage that it also works when the moduli $L_a$ are complex (Milton, 1987a, 1987b).

In the special case of a composite with $p = 2$ the strings of indices merely consist of a repeated string of either 2’s or 1’s (according to whether $q = 1$ or $q = 2$) terminated by a space index. Let us drop this redundant information and allow the elements of the weight and normalization matrices to be addressed only by the space indices. Also when $p = 2$ the matrices $\hat{\mathbf{W}}^j_1$ and $\hat{\mathbf{W}}^j_2$ commute and so we have

$$\hat{\mathbf{Y}}^j = \hat{\mathbf{W}}^j_1 \hat{\mathbf{W}}^j_2, \quad \hat{\mathbf{M}}^j = (\hat{\mathbf{W}}^j_1 \hat{\mathbf{W}}^j_2)^{1/2}, \quad \hat{\mathbf{Q}}^j_1 = \hat{\mathbf{W}}^j_2, \quad \hat{\mathbf{Q}}^j_2 = \hat{\mathbf{W}}^j_1.$$  

(10.1)

Without loss of generality we take $q = 2$, and correspondingly $L_0 = L_2$. Then the recursion relation (9.9) simplifies to

$$\hat{\mathbf{L}}^j-1 = \hat{\mathbf{W}}^j-1_1 \mathbf{L}_1 + \hat{\mathbf{W}}^j-1_2 \mathbf{L}_2 - (\mathbf{L}_1 - \mathbf{L}_2) \hat{\mathbf{M}}^j (\hat{\mathbf{W}}^j_1 \hat{\mathbf{W}}^j_2)^{1/2} + (\hat{\mathbf{N}}^j)^{1/2} (\hat{\mathbf{L}}^j)^{1/2} \hat{\mathbf{M}}^j (\hat{\mathbf{L}}^j)^{1/2} (\mathbf{L}_1 - \mathbf{L}_2),$$  

(10.2)
which for $L_1 \neq L_2$ can be inverted to give $\hat{L}^*j$ in terms of $\hat{L}^{*j-1}$:

\[
\hat{L}^*j = (\hat{N}^j)^{-1/2}\left\{-\hat{W}^j_1^{-1}L_2 - \hat{W}^j_2^{-1}L_1 + (L_1 - L_2)\hat{M}^j(\hat{W}^j_1^{-1}L_1 + \hat{W}^j_2^{-1}L_2 - \hat{L}^{*j-1})^{-1}\hat{M}^j(L_1 - L_2)\right\}(\hat{N}^j)^{-1/2}.
\]

(10.3)

Supposing that the components are isotropic phases occupying volume fractions $f_1$ and $f_2$, (4.20) implies

\[
W^0_{1,\alpha,\beta} = f_1\delta_{\alpha\beta}, \quad W^0_{2,\alpha,\beta} = f_2\delta_{\alpha\beta},
\]

(10.4)

and consequently when $j = 1$ (10.3) takes the form

\[
\hat{L}^{*1} = (\hat{N}^1)^{-1/2}\hat{Y}^*(\hat{N}^1)^{-1/2},
\]

(10.5)

where $\hat{Y}^*$, not to be confused with the matrix $\hat{Y}^j$, is given by

\[
\hat{Y}^* = -f_1 \hat{I} L_2 - f_2 \hat{I} L_1 + f_1 f_2 (L_1 - L_2)(f_1 \hat{I} L_1 + f_2 \hat{I} L_2 - \hat{L}^{*})^{-1}(L_1 - L_2).
\]

(10.6)

11 Bounds using the translation method

It turns out that bounds on $\hat{L}^*$ derived via the translation method follow from elementary bounds on this tensor $\hat{Y}^*$. This method was discovered independently by Murat and Tartar (1979;1985;1985) and by Lurie and Cherkaev (1982;1984) and applied to generate bounds that characterize for $n = 1$ the region in tensor space filled by the range of values $\hat{L}^*$ takes as the microstructure varies over all configurations while keeping the moduli $L_1$ and $L_2$ and the volume fraction $f_1$ fixed. Subsequently it was noted that the corresponding region filled by the possible values of $\hat{Y}^*$ did not depend on the choice of volume fraction $f_1$ (Milton 1986a). Cherkaev and Gibiansky (1992) extended the characterization to $n = 2$, assuming a two-dimensional geometry. Subsequently Clark and Milton (1995) obtained the characterization for arbitrary $n$, using fractional linear transformations which preserve the analytic properties as functions of the component moduli.

To explain the translation method let us focus on bounding $\hat{L}^*$ from below. Then one needs to find a suitable translation tensor $T_{\alpha i \beta k}$, where $i, k$ are field indices and $\alpha, \beta$ are space indices, satisfying

\[
\hat{I} L_a \geq \hat{T}, \quad a = 1, 2,
\]

(11.1)

and with the additional property that

\[
\int_{\Omega} d\vec{r} \nabla \psi \cdot \hat{T} \nabla \psi \geq 0,
\]

(11.2)

for all periodic potentials $\psi$ with elements $\psi^k(\vec{r}), k = 1, 2, \ldots n$. Any positive semidefinite tensor satisfies this last constraint. However the converse is not true, and in fact the interesting applications to bounds come from translations $\hat{T}$ which are not positive semidefinite. The key idea in the method is to consider a comparison composite with its moduli translated from $\hat{L}(\vec{r})$ to the moduli

\[
\hat{L}'(\vec{r}) \equiv \hat{L}(\vec{r}) - \hat{T},
\]

(11.3)
which are positive semidefinite as a consequence of (11.1). From (11.2) and from the variational
definition [9.1] applied to the effective tensor \( \hat{L}^* \) of the comparison composite we have, for all
uniform fields \( \vec{E}_0 \),

\[
\vec{E}_0 \cdot \hat{L}^* \vec{E}_0 = \min_\psi \left\{ \int_\Omega d\vec{r} \left( \vec{E}_0 - \vec{\nabla} \psi(\vec{r}) \right) \cdot \left( \hat{L}'(\vec{r}) \right) \left( \vec{E}_0 - \vec{\nabla} \psi(\vec{r}) \right) \right\}
\]

\[
= \min_\psi \left\{ \int_\Omega d\vec{r} \left( \vec{E}_0 - \vec{\nabla} \psi(\vec{r}) \right) \cdot \left( \hat{L}(\vec{r}) \right) \left( \vec{E}_0 - \vec{\nabla} \psi(\vec{r}) \right) \right. \\
- \left. \int_\Omega d\vec{r} \left( \vec{\nabla} \psi(\vec{r}) \right) \cdot \left( \hat{T}(\vec{r}) \right) \left( \vec{E}_0 - \vec{\nabla} \psi(\vec{r}) \right) - \vec{E}_0 \cdot \hat{T} \vec{E}_0 \right\}
\]

\[
\leq \min_\psi \left\{ \int_\Omega d\vec{r} \left( \vec{E}_0 - \vec{\nabla} \psi(\vec{r}) \right) \cdot \left( \hat{L}(\vec{r}) \right) \left( \vec{E}_0 - \vec{\nabla} \psi(\vec{r}) \right) \right\} - \vec{E}_0 \cdot \hat{T} \vec{E}_0
\]

\[
= \vec{E}_0 \cdot \left( \hat{L}^* - \hat{T} \right) \vec{E}_0,
\]

(11.4)

which is equivalent to the tensor inequality

\[
\hat{L}^* \leq \hat{L}^* - \hat{T}.
\]

(11.5)

Substituting this in the harmonic mean bounds on \( \hat{L}^* \),

\[
(\hat{L}^*)^{-1} \leq \int_\Omega d\vec{r} \left( \hat{L}'(\vec{r}) \right)^{-1},
\]

(11.6)

yields the translation bounds,

\[
\left( \hat{L}^* - \hat{T} \right)^{-1} \leq \int_\Omega d\vec{r} \left( \hat{L}(\vec{r}) - \hat{T} \right)^{-1},
\]

(11.7)

which for composites of two isotropic materials reduces to

\[
\left( \hat{L}^* - \hat{T} \right)^{-1} \leq f_1 \left( \hat{I} L_1 - \hat{T} \right)^{-1} + f_2 \left( \hat{I} L_2 - \hat{T} \right)^{-1}.
\]

(11.8)

Cherkaev and Gibiansky (1992) noticed through algebraic manipulation, that these bounds
when expressed in terms of \( \hat{Y}^* \) simplify to

\[
\hat{Y}^* + \hat{T} \geq 0.
\]

(11.9)

In their proof they assumed that \( L_1 \) and \( L_2 \) commute. Later this assumption was found
unnecessary and moreover a direct and simple proof of (11.9) was found from a variational
expression for \( \hat{Y}^* \) (Milton 1991). An interesting feature of the translation method is that the
sharpest bounds are usually obtained from translations \( \hat{T} \) with couplings between the fields,
even when \( L_1 \) and \( L_2 \), and hence \( \hat{L}^* \), have no such couplings.

When \( p > 2 \) the transformation (9.9) cannot simply be inverted because the matrices \( \hat{M}_a^j \)
are rectangular and have no unique inverse. Also it is clear that the tensor \( \hat{L}^* \) is larger than
the tensor \( \hat{L}^{*j} \) and so contains more information. However if more than one field was present,
i.e. if \( n \geq 2 \), and if \( \hat{L}^* \) was known as a function of the \( L_a \), then in principle one could expand
\( \hat{L}^* \) in a power series, possibly extract the coefficients \( \hat{a}_{a_1...a_n} \) and subsequently find the weights
and normalization matrices. By this means one could recover both \( \hat{L}^* \) and

\[
\hat{Y}^* = (\hat{N}^j)^{-1/2} \hat{L}^* \hat{N}^j (\hat{N}^j)^{-1/2}
\]

(11.10)
as a function of the $\mathbf{L}_a$ through the continued fraction formula for $\mathbf{\tilde{Y}}^{sj}$ implied by (9.9). Naturally we expect that there exists a more direct way of recovering the function $\mathbf{\tilde{Y}}^{sj}(\mathbf{L}_1, \mathbf{L}_2, ..., \mathbf{L}_p)$ from the function $\mathbf{\tilde{L}}^{sj-1}(\mathbf{L}_1, \mathbf{L}_2, ..., \mathbf{L}_p)$. One intriguing question is whether this direct recovery process, whatever it is, works when $n = 1$. If it does then the sequence of matrices $\mathbf{\tilde{N}}^j$ and $\mathbf{\tilde{W}}_a^j$ could be recovered by expanding each function $\mathbf{\tilde{Y}}^{sj-1}(\mathbf{L}_1, \mathbf{L}_2, ..., \mathbf{L}_p)$ to first order, and consequently $\mathbf{\tilde{L}}^*$ could be calculated even when more than one field is present. In other words, knowledge of the conductivity function $\mathbf{\sigma}^{*j}(\sigma_1, \sigma_2, ..., \sigma_p)$ without couplings would be sufficient to uniquely determine the effective tensor $\mathbf{\tilde{L}}^*$ with couplings present.

Acknowledgments

This manuscript was largely complete in 1992, and at that time Graeme W. Milton was an associate professor at the Courant Institute, and a recipient of a Packard Fellowship, and Mordehai Milgrom was a visitor to the Courant Institute. Conversely Graeme W. Milton benefited from a visit to the Weizmann Institute. The Courant Institute, the Packard Foundation, the University of Utah, and the Weizmann Institute are gratefully thanked for their support.

References

Allaire, G. 2002. *Shape optimization by the homogenization method*. Berlin / Heidelberg / London / etc.: Springer-Verlag. 456 pp.

Bensoussan, A., J.-L. Lions, and G. Papanicolaou 1978. *Asymptotic Analysis for Periodic Structures*. Amsterdam: North-Holland Publishing Co. xxiv + 700 pp. ISBN 0-444-85172-0. LCCN QA379 .B45.

Beran, M. J. 1965. Use of the variational approach to determine bounds for the effective permittivity in random media. *Nuovo Cimento* 38(2):771–782.

Beran, M. J. 1968. *Statistical Continuum Theories*. New York: Interscience Publishers. xv + 424 pp. ISBN 0-470-06861-2. LCCN QA808.2 B47 1968.

Beran, M. J. and J. J. McCoy 1970. Mean field variations in a statistical sample of heterogeneous linear elastic solids. *International Journal of Solids and Structures* 6:1035–1054.

Beran, M. J. and J. Molyneux 1963. Statistical properties of the electric field in a medium with small random variations in permittivity. *Nuovo Cimento* 30:1406–1422.

Beran, M. J. and J. Molyneux 1966. Use of classical variational principles to determine bounds for the effective bulk modulus in heterogeneous media. *Quarterly of Applied Mathematics* 24:107–118.

Brown, W. F. 1955. Solid mixture permittivities. *Journal of Chemical Physics* 23:1514–1517.

Bruno, O. P. 1991. Taylor expansions and bounds for the effective conductivity and the effective elastic moduli of multicomponent composites and polycrystals. *Asymptotic Analysis* 4(4):339–365.

Cherkaev, A. V. 2000. *Variational Methods for Structural Optimization*. Berlin / Heidelberg / London / etc.: Springer-Verlag. xxvi + 545 pp. ISBN 0-387-98462-3. LCCN QA1.A647 vol. 140.
Cherkaev, A. V. and L. V. Gibiansky 1992. The exact coupled bounds for effective tensors of electrical and magnetic properties of two-component two-dimensional composites. *Proceedings of the Royal Society of Edinburgh. Section A, Mathematical and Physical Sciences* 122(1–2):93–125.

Clark, K. E. and G. W. Milton 1994. Modeling the effective conductivity function of an arbitrary two-dimensional polycrystal using sequential laminates. *Proceedings of the Royal Society of Edinburgh* 124A(4):757–783.

Clark, K. E. and G. W. Milton 1995. Optimal bounds correlating electric, magnetic and thermal properties of two-phase, two-dimensional composites. *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences* 448:161–190.

Dederichs, P. H. and R. Zeller 1973. Variational treatment of the elastic constants of disordered materials. *Zeitschrift für Physik* 259:103–116.

Dykhne, A. M. 1970. Conductivity of a two-dimensional two-phase system. *Zhurnal eksperimental’noi i teoreticheskoi fiziki / Akademiia Nauk SSSR* 59:110–115. English translation in *Soviet Physics JETP* 32:63–65 (1971).

Fokin, A. G. and T. D. Shermergor 1969. Calculation of effective elastic moduli of composite materials with multiphase interactions taken into account. *Journal of Applied Mechanics and Technical Physics* 10:48–54.

Gilbarg, D. and N. S. Trudinger 1983. *Elliptic Partial Differential Equations of Second Order*. Berlin / Heidelberg / London / etc.: Springer-Verlag. 513 pp. ISBN 3-540-13025. LCCN QA377.G49 1983.

Golden, K. and G. Papanicolaou 1983. Bounds for effective parameters of heterogeneous media by analytic continuation. *Communications in Mathematical Physics* 90(4):473–491.

Gubernatis, J. E. and J. A. Krumhansl 1975. Macroscopic engineering properties of polycrystalline materials: Elastic properties. *Journal of Applied Physics* 46:1875–1883.

Hashin, Z. and S. Shtrikman 1962. A variational approach to the theory of the effective magnetic permeability of multiphase materials. *Journal of Applied Physics* 33:3125–3131.

Herring, C. 1960. Effect of random inhomogeneities on electrical and galvanomagnetic measurements. *Journal of Applied Physics* 31(11):1939–1953.

Hori, M. 1973. Statistical theory of effective electrical, thermal, and magnetic properties of random heterogeneous materials. I. Perturbation expansions for the effective permittivity of cell materials. *Journal of Mathematical Physics* 14(4):514–523.

Keller, J. B. 1964. A theorem on the conductivity of a composite medium. *Journal of Mathematical Physics* 5(4):548–549.

Kozlov, S. M. 1978. Averaging of random structures. *Doklady Akademii Nauk SSSR* 241(5):1016–1019. English translation in *Soviet Math. Dokl.* 19(4):950–954 (1978).

Kröner, E. 1977. Bounds for the effective elastic moduli of disordered materials. *Journal of the Mechanics and Physics of Solids* 25:137–155.

Lurie, K. A. and A. V. Cherkaev 1982. Accurate estimates of the conductivity of mixtures formed of two materials in a given proportion (two-dimensional problem). *Doklady Akademii Nauk SSSR* 264:1128–1130. English translation in *Soviet Phys. Dokl.* 27:461–462 (1982).
Lurie, K. A. and A. V. Cherkaev 1984. Exact estimates of conductivity of composites formed by two isotropically conducting media taken in prescribed proportion. *Proceedings of the Royal Society of Edinburgh. Section A, Mathematical and Physical Sciences* 99(1–2):71–87.

McPhedran, R. C. and G. W. Milton 1981. Bounds and exact theories for the transport properties of inhomogeneous media. *Applied Physics A* 26:207–220.

Mendelson, K. S. 1975. A theorem on the effective conductivity of a two-dimensional heterogeneous medium. *Journal of Applied Physics* 46(11):4740–4741.

Meyers, N. G. 1963. An $L^p$-estimate for the gradient of solutions of second order elliptic divergence form equations. *Annali della Scuola Normale Superiore di Pisa. Serie III* 17(3):189–206.

Milgrom, M. 1990. Linear response of general composite systems to many coupled fields. *Physical Review B (Solid State)* 41(18):12484–12494.

Milton, G. W. 1981. Bounds on the transport and optical properties of a two-component composite material. *Journal of Applied Physics* 52(8):5294–5304.

Milton, G. W. 1986b. A proof that laminates generate all possible effective conductivity functions of two-dimensional, two-phase media. In G. Papanicolaou (ed.), *Advances in Multiphase Flow and Related Problems: Proceedings of the Workshop on Cross Disciplinary Research in Multiphase Flow, Leesburg, Virginia, June 2–4, 1986*, pp. 136–146. Philadelphia: SIAM Press. ISBN 0-89871-212-2. LCCN QA922 .W671 1986.

Milton, G. W. 1986a. Modeling the properties of composites by laminates. In J. L. Ericksen, D. Kinderlehrer, R. Kohn, and J.-L. Lions (eds.), *Homogenization and Effective Moduli of Materials and Media*, pp. 150–174. Berlin / Heidelberg / London / etc.: Springer-Verlag. ISBN 0-387-96306-5. LCCN QA808.2 .H661 1986.

Milton, G. W. 1987a. Multicomponent composites, electrical networks and new types of continued fraction. I. *Communications in Mathematical Physics* 111(2):281–327.

Milton, G. W. 1987b. Multicomponent composites, electrical networks and new types of continued fraction. II. *Communications in Mathematical Physics* 111(3):329–372.

Milton, G. W. 1991. The field equation recursion method. In G. Dal Maso and G. F. Dell’Antonio (eds.), *Composite Media and Homogenization Theory: Proceedings of the Workshop on Composite Media and Homogenization Theory Held in Trieste, Italy, from January 15 to 26, 1990*, pp. 223–245. Basel, Switzerland: Birkhäuser Verlag. ISBN 0-8176-3511-4, 3-7643-3511-4. LCCN QA808.2 .C665 1991.

Milton, G. W. 2002. *The Theory of Composites*. Cambridge, United Kingdom: Cambridge University Press. xxviii + 719 pp. ISBN 0-521-78125-6. LCCN TA418.9.C6M58 2001.

Milton, G. W. and K. Golden 1985. Thermal conduction in composites. In T. Ashworth and D. R. Smith (eds.), *Thermal Conductivity*, pp. 571–582. New York / London: Plenum Press. ISBN 0-306-41918-1. LCCN QC 320.8 I58 1983.

Milton, G. W. and R. C. McPhedran 1982. A comparison of two methods for deriving bounds on the effective conductivity of composites. In R. Burridge, S. Childress, and G. Papanicolaou (eds.), *Macroscopic Properties of Disordered Media: Proceedings of a Conference Held at the Courant Institute, June 1–3, 1981*, pp. 183–193. Berlin / Heidelberg / London / etc.: Springer-Verlag. ISBN 0-387-11202-2. LCCN QA911 .M32 1981.

Milton, G. W. and N. Phan-Thien 1982. New bounds on effective elastic moduli of two-component materials. *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences* 380:305–331.
Murat, F. and L. Tartar 1985. Calcul des variations et homogénéisation. (French) [Calculus of variation and homogenization]. In Les méthodes de l’homogénéisation: théorie et applications en physique, pp. 319–369. Paris: Eyrolles. English translation in Topics in the Mathematical Modelling of Composite Materials, pp. 139–173, ed. by A. Cherkaev and R. Kohn, ISBN 0-8176-3662-5. LCCN QC20.5 .M47 1985; TA418.9.C6 M473 1985.

Phan-Thien, N. and G. W. Milton 1982. New bounds on the effective thermal conductivity of N-phase materials. Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences 380:333–348.

Phan-Thien, N. and G. W. Milton 1983. New third-order bounds on the effective moduli of N-phase composites. Quarterly of Applied Mathematics 41:59–74.

Prager, S. 1960. Diffusion in inhomogeneous media. Journal of Chemical Physics 33(1):122–127.

Sen, A. K. and S. Torquato 1989. Effective conductivity of anisotropic two-phase composite media. Physical Review B 39(7):4504–4515.

Strang, G. 1986. Introduction to Applied Mathematics, pp. 414–419. Wellesley, Massachusetts: Wellesley-Cambridge Press. ISBN 0-9614088-0-4. LCCN QA37 .2 .S871 1986.

Tartar, L. 1979. Estimation de coefficients homogénéisés. (French) [Estimation of homogenization coefficients]. In R. Glowinski and J.-L. Lions (eds.), Computing Methods in Applied Sciences and Engineering: Third International Symposium, Versailles, France, December 5–9, 1977, pp. 364–373. Berlin / Heidelberg / London / etc.: Springer-Verlag, English translation in Topics in the Mathematical Modelling of Composite Materials, pp. 9–20, ed. by A. Cherkaev and R. Kohn. ISBN 0-8176-3662-5. ISBN 0-387-09123-8.

Tartar, L. 1985. Estimations fines des coefficients homogénéisés. (French) [Fine estimations of homogenized coefficients]. In P. Krée (ed.), Ennio de Giorgi Colloquium: Papers Presented at a Colloquium Held at the H. Poincaré Institute in November 1983, pp. 168–187. London: Pitman Publishing Ltd. ISBN 0-273-08680-4. LCCN QA377 .E56 1983.

Tartar, L. 1989. H-measures and small amplitude homogenization. In R. V. Kohn and G. W. Milton (eds.), Proceedings of the SIAM Workshop on Random Media and Composites, Leesburg, Virginia, December 7–10, 1988, pp. 89–99. Philadelphia: SIAM Press. ISBN 0-89871-246-7. LCCN TA401.3 .S53 1988.

Tartar, L. 1990. H-measures, a new approach for studying homogenization, oscillations and concentration effects in partial differential equations. Proceedings of the Royal Society of Edinburgh. Section A, Mathematical and Physical Sciences 115(3–4):193–230.

Tartar, L. 2009. The General Theory of Homogenization: A Personalized Introduction. Berlin / Heidelberg / London / etc.: Springer-Verlag. ISBN 978-3-642-05194-4.

Torquato, S. 1997. Effective stiffness tensor of composite media. I. Exact series expansions. Journal of the Mechanics and Physics of Solids 45(9):1421–1448.

Torquato, S. 2002. Random Heterogeneous Materials: Microstructure and Macroscopic Properties. Berlin / Heidelberg / London / etc.: Springer-Verlag. 703 pp. ISBN 978-0-387-95167-6.

Wiener, O. 1912. Die Theorie des Mischkörpers für das Feld des stationären Strömung. Erste Abhandlung die Mittelwertsätze für Kraft, Polarisation und Energie. (German) [The theory of composites for the field of steady flow. First treatment of mean value estimates for force, polarization and energy]. Abhandlungen der mathematisch-physischen Klasse der Königlich Sächsischen Gesellschaft der Wissenschaften 32:509–604.
Willis, J. R. 1977. Bounds and self-consistent estimates for the overall properties of anisotropic composites. *Journal of the Mechanics and Physics of Solids* 25:185–202.

Willis, J. R. 1981. Variational and related methods for the overall properties of composites. *Advances in Applied Mechanics* 21:1–78.

Zeller, R. and P. H. Dederichs 1973. Elastic constants of polycrystals. *Physica Status Solidi. B, Basic Research* 55:831–842.

Zhikov, V. V., S. M. Kozlov, and O. A. Oleinik 1994. *Homogenization of Differential Operators and Integral Functionals*. Berlin / Heidelberg / London / etc.: Springer-Verlag. xi + 570 pp. ISBN 3-540-54809-2 (Berlin), 0-387-54809-2 (New York). LCCN QA377 .Z45 1994.