Exact relations for composites: towards a complete solution

Yury Grabovsky and Graeme W. Milton[1]

Abstract. Typically, the electrical and elastic properties of composite materials are strongly microstructure dependent. So it comes as a nice surprise to come across exact formulae for (or linking) effective tensor elements that are universally valid no matter what the microstructure. Here we present a systematic theory of exact relations embracing the known exact relations and establishing new ones. The search for exact relations is reduced to a search for tensor subspaces satisfying certain algebraic conditions. One new exact relation is for the effective shear modulus of a class of three-dimensional polycrystalline materials.

1991 Mathematics Subject Classification: Primary 35B27, 73B27, 73S10; Secondary 73B40, 49J45
Keywords and Phrases: Composites, homogenization, polycrystals, exact relations

Introduction

Take a metal rod. We can bend it, twist it, stretch it, vibrate it or use it as a conduit for the flow of electrons or heat. It looks just like a homogeneous material with behavior governed by bulk and shear elastic moduli and electrical and thermal conductivities. However if we break the metal rod there is a surprise! One can see that the surface of the break is rough, comprised of individual crystalline grains sparkling in the light. Similarly foam rubber behaves like a highly compressible homogeneous elastic material, even though its pore structure is quite complicated. Homogenization theory provides a rigorous mathematical basis for the observation that materials with microstructure can effectively behave like homogeneous materials on a macroscopic scale. A typical result is the following. To ensure ellipticity of the equations let us suppose we are given positive constants α and $\beta > \alpha$ and a periodic conductivity tensor field $\boldsymbol{\sigma}(\boldsymbol{x})$ taking values in the set $\mathcal{M}_c$ comprising of all $d \times d$ symmetric matrices $\boldsymbol{\sigma}$ satisfying

$$\alpha \boldsymbol{v} \cdot \boldsymbol{v} \leq \boldsymbol{v} \cdot \boldsymbol{\sigma} \boldsymbol{v} \leq \beta \boldsymbol{v} \cdot \boldsymbol{v}, \tag{1}$$

[1]Both authors are supported by the National Science Foundation through grants DMS9402763, DMS9629692, DMS9704813 and DMS-9803748.

for all vectors $\boldsymbol{v}$. Then with $\boldsymbol{\sigma}_\epsilon(\boldsymbol{x}) = \boldsymbol{\sigma}(\boldsymbol{x}/\epsilon)$ the electrical potential $\phi_\epsilon(\boldsymbol{x})$ which solves the Dirichlet problem

$$\nabla \cdot \boldsymbol{\sigma}_\epsilon(\boldsymbol{x})\nabla\phi_\epsilon(\boldsymbol{x}) = f(\boldsymbol{x}) \ \text{ within } \ \Omega, \quad \phi_\epsilon(\boldsymbol{x}) = \psi(\boldsymbol{x}) \ \text{ on } \partial\Omega, \tag{2}$$

converges as $\epsilon \to 0$ (i.e. as the length scale of the periodicity of $\boldsymbol{\sigma}_\epsilon(\boldsymbol{x})$ shrinks to zero) to the potential ϕ_0 which solves

$$\nabla \cdot \boldsymbol{\sigma}_*\nabla\phi_0(\boldsymbol{x}) = f(\boldsymbol{x}) \ \text{ within } \ \Omega, \quad \phi_0(\boldsymbol{x}) = \psi(\boldsymbol{x}) \ \text{ on } \partial\Omega, \tag{3}$$

where the effective conductivity tensor $\boldsymbol{\sigma}_*$ is in $\mathcal{M}_c$ and only depends on $\boldsymbol{\sigma}(\boldsymbol{x})$ and not upon the choice of Ω, the source term $f(\boldsymbol{x})$, nor upon the potential $\psi(\boldsymbol{x})$ prescribed at the boundary. The effective conductivity tensor $\boldsymbol{\sigma}_*$ is obtained by solving the following *cell-problem.* One looks for periodic vector fields $\boldsymbol{j}(\boldsymbol{x})$ and $\boldsymbol{e}(\boldsymbol{x})$, representing the current and electric fields, which satisfy

$$\boldsymbol{j}(\boldsymbol{x}) = \boldsymbol{\sigma}(\boldsymbol{x})\boldsymbol{e}(\boldsymbol{x}), \qquad \nabla \cdot \boldsymbol{j} = 0, \qquad \nabla \times \boldsymbol{e} = 0. \tag{4}$$

The relation $\langle \boldsymbol{j} \rangle = \boldsymbol{\sigma}_*\langle \boldsymbol{e} \rangle$ between the average current and electric fields serves to define $\boldsymbol{\sigma}_*$. Here, as elsewhere, the angular brackets will be used to denote volume averages over the unit cell of periodicity. Homogenization results extend to fields $\boldsymbol{\sigma}_\epsilon(\boldsymbol{x})$ taking values in $\mathcal{M}_c$ which are locally periodic, or random and stationary, or simply arbitrary: see Bensoussan, et. al. (1978), Zhikov, et. al. (1994), and Murat and Tartar (1997) and references therein.

Similar results hold for elasticity. Given positive constants α and $\beta > \alpha$ and a periodic elasticity tensor field $\boldsymbol{\mathcal{C}}(\boldsymbol{x})$ taking values in the set $\mathcal{M}_e$ comprised of all elasticity tensors $\boldsymbol{\mathcal{C}}$ satisfying

$$\alpha \boldsymbol{A} \cdot \boldsymbol{A} \leq \boldsymbol{A} \cdot \boldsymbol{\mathcal{C}}\boldsymbol{A} \leq \beta \boldsymbol{A} \cdot \boldsymbol{A}, \tag{5}$$

for all symmetric $d \times d$ matrices $\boldsymbol{A}$, there is an associated effective elasticity tensor $\boldsymbol{\mathcal{C}}_*$ in $\mathcal{M}_e$. It is obtained by looking for periodic symmetric matrix valued fields $\boldsymbol{\tau}(\boldsymbol{x})$ and $\boldsymbol{\epsilon}(\boldsymbol{x})$, representing the stress and strain fields, which satisfy

$$\boldsymbol{\tau}(\boldsymbol{x}) = \boldsymbol{\mathcal{C}}(\boldsymbol{x})\boldsymbol{\epsilon}(\boldsymbol{x}), \qquad \nabla \cdot \boldsymbol{\tau} = 0, \quad \boldsymbol{\epsilon} = [\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T]/2, \tag{6}$$

in which $\boldsymbol{u}(\boldsymbol{x})$ represents the displacement field. The relation $\langle \boldsymbol{\tau} \rangle = \boldsymbol{\mathcal{C}}_*\langle \boldsymbol{\epsilon} \rangle$ between the average stress and strain fields serves to define $\boldsymbol{\mathcal{C}}_*$.

A key problem, of considerable technological importance, is to determine the effective tensors $\boldsymbol{\sigma}_*$ and $\boldsymbol{\mathcal{C}}_*$ governing the behaviour on the macroscopic scale. For a long while it was the dream of many experimentalists and theorists alike that there should be some universally applicable "mixing formula" giving the effective tensors as some sort of average of the tensors of the crystalline grains or constituent materials. However the reality is that the details of the microgeometry can sometimes play an influential role in determining the overall properties, particularly when the crystalline grains have highly anisotropic behavior or when there is a large contrast in the properties of the constituent materials. Consider, for example, a two-phase composite where one phase is rigid and the second phase is compressible. The question of whether the composite as a whole is rigid or compressible is not solely determined by the volume fractions occupied by the phases, but depends on whether the rigid phase has a connected component spanning the material or consists of isolated inclusions embedded in the compressible phase.

So we have to temper the dream. Instead of seeking a universally applicable "mixing formula" one can ask whether certain combinations of effective tensor elements can be microstructure independent. Indeed they can. Sometimes these exact relations are easy to deduce and sometimes they are not at all obvious. Such exact relations provide useful benchmarks for testing approximation schemes and numerical calculations of effective tensors. Grabovsky (1998) recognized that there should be some general theory of exact relations. Utilizing the fact that an exact relation must hold for laminate materials he derived restrictive constraints on the form that an exact relation can take. This reduced the search for candidate exact relation to an algebraic question that was analysed by Grabovsky and Sage (1998). Here we give sufficient conditions for an exact relation to hold for all composite microgeometries, and not just laminates. At present the general theory of exact relations is still not complete. There is a gap between the known necessary conditions and the known sufficient conditions for an exact relation to hold. In addition the associated algebraic questions have only begun to be investigated. Before proceeding to the general theory let us first look at some examples: see also the recent review of Milton (1997).

Examples of some elementary exact relations

An example of a relation which is easy to deduce is the following. Lurie, Cherkaev and Fedorov (1984) noticed that if the elasticity tensor field $\boldsymbol{\mathcal{C}}(\boldsymbol{x})$ is such that there exist non-zero symmetric tensors $\boldsymbol{V}$ and $\boldsymbol{W}$ with $\boldsymbol{\mathcal{C}}(\boldsymbol{x})\boldsymbol{V} = \boldsymbol{W}$ for all $\boldsymbol{x}$ then the effective tensor $\boldsymbol{\mathcal{C}}_*$ must satisfy $\boldsymbol{\mathcal{C}}_*\boldsymbol{V} = \boldsymbol{W}$. The reason is simply that the elastic equations are solved with a constant strain $\boldsymbol{\epsilon}(\boldsymbol{x}) = \boldsymbol{V}$ and a constant stress $\boldsymbol{\tau}(\boldsymbol{x}) = \boldsymbol{W}$ and the effective tensor, by definition, relates the averages of these two fields. In particular, consider a single phase polycrystalline material, where the crystalline phase has cubic symmetry. Each individual crystal responds isotropically to hydrostatic compression, and we can take $\boldsymbol{V} = \boldsymbol{I}$ and $\boldsymbol{W} = d\kappa_0\boldsymbol{I}$ where d is the spatial dimension (2 or 3) and κ_0 is the bulk modulus of the pure crystal. The result implies that the effective bulk modulus κ_* of the polycrstal is κ_0 (Hill, 1952). Another way of expressing this exact relation is to introduce the manifold

$$\mathcal{M} = \mathcal{M}(\boldsymbol{V}, \boldsymbol{W}) = \{\boldsymbol{\mathcal{C}} \in \mathcal{M}_e \mid \boldsymbol{\mathcal{C}}\boldsymbol{V} = \boldsymbol{W}\}, \tag{7}$$

of elasticity tensors. The exact relation says that if $\boldsymbol{\mathcal{C}}(\boldsymbol{x}) \in \mathcal{M}$ for all $\boldsymbol{x}$ then $\boldsymbol{\mathcal{C}}_* \in \mathcal{M}$. In other words the manifold $\mathcal{M}$ is stable under homogenization. It defines an exact relation because it has no interior. Many other important exact relations derive from uniform field arguments: see Dvorak and Benveniste (1997) and references therein.

The classic example of a non-trivial exact relation is for two-dimensional conductivity (or equivalently for three-dimensional conductivity with microstructure independent of one coordinate). When $d = 2$ the equations (4) can be written in the equivalent form

$$\boldsymbol{j}'(\boldsymbol{x}) = \boldsymbol{\sigma}'(\boldsymbol{x})\boldsymbol{e}'(\boldsymbol{x}), \quad \nabla\cdot\boldsymbol{j}'(\boldsymbol{x}) = 0, \quad \nabla\times\boldsymbol{e}'(\boldsymbol{x}) = 0, \tag{8}$$

where

$$\boldsymbol{j}'(\boldsymbol{x}) \equiv c\boldsymbol{R}_\perp\boldsymbol{e}(\boldsymbol{x}), \quad \boldsymbol{e}'(\boldsymbol{x}) \equiv \boldsymbol{R}_\perp\boldsymbol{j}(\boldsymbol{x}), \quad \boldsymbol{\sigma}'(\boldsymbol{x}) \equiv c\boldsymbol{R}_\perp[\boldsymbol{\sigma}(\boldsymbol{x})]^{-1}\boldsymbol{R}_\perp^T. \tag{9}$$

in which c is a constant and $\boldsymbol{R}_\perp$ is the matrix for a $90°$ rotation. In other words the fields $\boldsymbol{j}'(\boldsymbol{x})$ and $\boldsymbol{e}'(\boldsymbol{x})$ solve the conductivity equations in a medium with conductivity $\boldsymbol{\sigma}'(\boldsymbol{x})$. Moreover by looking at the relations satisfied by the average fields one sees that the effective conductivity tensor $\boldsymbol{\sigma}'_*$ associated with $\boldsymbol{\sigma}'(\boldsymbol{x})$ and the effective conductivity tensor $\boldsymbol{\sigma}'_*$ associated with $\boldsymbol{\sigma}(\boldsymbol{x})$ are linked by the relation

$$\boldsymbol{\sigma}'_* = c\boldsymbol{R}_\perp(\boldsymbol{\sigma}_*)^{-1}\boldsymbol{R}_\perp^T, \tag{10}$$

[see Keller (1964), Dykhne (1970) and Mendelson (1975)]. Now suppose the conductivity tensor field is such that its determinant is independent of $\boldsymbol{x}$, i.e. $\det\boldsymbol{\sigma}(\boldsymbol{x}) = \Delta$. With $c = \Delta$ we have $\boldsymbol{\sigma}'(\boldsymbol{x}) = \boldsymbol{\sigma}(\boldsymbol{x})$ implying $\boldsymbol{\sigma}'_* = \boldsymbol{\sigma}_*$. From (10) one concludes that $\det\boldsymbol{\sigma}_* = \Delta$. In other words the manifold

$$\mathcal{M} = \mathcal{M}(\Delta) = \{\boldsymbol{\sigma}\in\mathcal{M}_c \mid \det\boldsymbol{\sigma} = \Delta\} \tag{11}$$

is stable under homogenization (Lurie and Cherkaev, 1981). Again it defines an exact relation because it has no interior. An important application of this result is to a single phase polycrystalline material where the crystalline phase has a conductivity tensor with determinant Δ. If the polycrystal has an isotropic conductivity tensor the exact relation implies the result of Dykhne (1970) that $\boldsymbol{\sigma}_* = \sqrt{\Delta}\boldsymbol{I}$.

An equation satisfied by the polarization field

For simplicity, let us consider the conductivity problem and take as our reference conductivity tensor a matrix $\boldsymbol{\sigma}_0$ in $\mathcal{M}_c$. Affiliated with $\boldsymbol{\sigma}_0$ is a non-local operator $\boldsymbol{\Gamma}$ defined as follows. Given any periodic vector-valued field $\boldsymbol{p}(\boldsymbol{x})$ we say that $\boldsymbol{e}' = \boldsymbol{\Gamma}\boldsymbol{p}$ if $\boldsymbol{e}'$ is curl-free with $\langle\boldsymbol{e}'\rangle = 0$ and $\boldsymbol{p} - \boldsymbol{\sigma}_0\boldsymbol{e}'$ is divergence-free. Equivalently, we have

$$\begin{aligned} \widehat{\boldsymbol{e}}'(\boldsymbol{k}) &= \boldsymbol{\Gamma}(\boldsymbol{k})\widehat{\boldsymbol{p}}(\boldsymbol{k}) \ \text{ for } \boldsymbol{k}\neq 0, \\ &= 0 \quad \text{when } \boldsymbol{k} = 0, \end{aligned} \tag{12}$$

where $\widehat{\boldsymbol{e}}'(\boldsymbol{k})$ and $\widehat{\boldsymbol{p}}(\boldsymbol{k})$ are the Fourier coefficients of $\boldsymbol{e}'(\boldsymbol{x})$ and $\boldsymbol{p}(\boldsymbol{x})$ and

$$\boldsymbol{\Gamma}(\boldsymbol{k}) = \frac{\boldsymbol{k}\otimes\boldsymbol{k}}{\boldsymbol{k}\cdot\boldsymbol{\sigma}_0\boldsymbol{k}}. \tag{13}$$

Now suppose we take a polarization field $\boldsymbol{p}(\boldsymbol{x}) = (\boldsymbol{\sigma}(\boldsymbol{x}) - \boldsymbol{\sigma}_0)\boldsymbol{e}(\boldsymbol{x})$ where $\boldsymbol{e}(\boldsymbol{x})$ solves the conductivity equations. It is analogous to the polarization field introduced in dielectric problems. From the definition (13) of the operator $\boldsymbol{\Gamma}$ we see immediately that it solves the equation

$$[\boldsymbol{I} + (\boldsymbol{\sigma} - \boldsymbol{\sigma}_0)\boldsymbol{\Gamma}]\boldsymbol{p} = (\boldsymbol{\sigma} - \boldsymbol{\sigma}_0)\langle\boldsymbol{e}\rangle \ \text{ and } \langle\boldsymbol{p}\rangle = (\boldsymbol{\sigma}_* - \boldsymbol{\sigma}_0)\langle\boldsymbol{e}\rangle. \tag{14}$$

For investigating exact relations it proves convenient to use another form of these equations. We choose a fixed matrix $\boldsymbol{M}$, define the fractional linear transformation

$$W_{\boldsymbol{M}}(\boldsymbol{\sigma}) = [\boldsymbol{I} + (\boldsymbol{\sigma} - \boldsymbol{\sigma}_0)\boldsymbol{M}]^{-1}(\boldsymbol{\sigma} - \boldsymbol{\sigma}_0), \tag{15}$$

(in which we allow for $\boldsymbol{\sigma} - \boldsymbol{\sigma}_0$ to be singular) and rewrite (14) as

$$[\boldsymbol{I} - \boldsymbol{K}\boldsymbol{A}]\boldsymbol{p} = \boldsymbol{K}\boldsymbol{v}, \quad \langle \boldsymbol{p} \rangle = \boldsymbol{K}_*\boldsymbol{v}, \tag{16}$$

where

$$\boldsymbol{K}(\boldsymbol{x}) = W_{\boldsymbol{M}}(\boldsymbol{\sigma}(\boldsymbol{x})), \quad \boldsymbol{K}_* = W_{\boldsymbol{M}}(\boldsymbol{\sigma}_*), \quad \boldsymbol{v} = \langle \boldsymbol{e} \rangle + \boldsymbol{M}\langle \boldsymbol{p} \rangle, \tag{17}$$

and $\boldsymbol{A}$ is the non-local operator defined by its action, $\boldsymbol{A}\boldsymbol{p} = \boldsymbol{M}(\boldsymbol{p} - \langle \boldsymbol{p} \rangle) - \boldsymbol{\Gamma}\boldsymbol{p}$. The formula (16) involves the operator $\boldsymbol{K}\boldsymbol{A}$. If $\boldsymbol{q} = \boldsymbol{K}\boldsymbol{A}\boldsymbol{p}$ we have

$$\boldsymbol{q}(\boldsymbol{x}) = \sum_{\boldsymbol{k}\neq 0} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\boldsymbol{K}(\boldsymbol{x})\boldsymbol{A}(\boldsymbol{k})\widehat{\boldsymbol{p}}(\boldsymbol{k}), \quad \text{where} \quad \boldsymbol{A}(\boldsymbol{k}) = \boldsymbol{M} - \boldsymbol{\Gamma}(\boldsymbol{k}), \tag{18}$$

and $\widehat{\boldsymbol{p}}(\boldsymbol{k})$ is the Fourier component of $\boldsymbol{p}(\boldsymbol{x})$.

Necessary conditions for an exact relation

Since exact relations hold for all microstructures they must in particular hold for laminate microstructures for which the tensors and hence the fields only have variations in one direction, $\boldsymbol{n}$. This simple consideration turns out to impose very stringent constraints. Consider the conductivity problem. Let us take $\boldsymbol{M} = \boldsymbol{\Gamma}(\boldsymbol{n})$ and let $W_{\boldsymbol{n}}(\boldsymbol{\sigma})$ denote the transformation $W_{\boldsymbol{M}}(\boldsymbol{\sigma})$. When $\boldsymbol{K}(\boldsymbol{x}) = \boldsymbol{K}(\boldsymbol{n}\cdot\boldsymbol{x})$ (16) is easily seen to have the solution $\boldsymbol{p}(\boldsymbol{x}) = \boldsymbol{K}(\boldsymbol{x})\boldsymbol{v}$ and $\boldsymbol{K}_* = \langle \boldsymbol{K} \rangle$ because $\boldsymbol{A}$ annihilates any field which only has oscillations in the direction $\boldsymbol{n}$. [Milton (1990) and Zhikov (1991) give related derivations of the formula $\boldsymbol{K}_* = \langle \boldsymbol{K} \rangle$: see also Backus (1962) and Tartar (1976) for other linear lamination formulae.] Since $\boldsymbol{K}_*$ is just a linear average of $\boldsymbol{K}(\boldsymbol{x})$ any set of conductivity tensors which is stable under homogenization, and hence lamination, must have a convex image under the transformation $W_{\boldsymbol{n}}$. In particular if a manifold $\mathcal{M}$ defines an exact relation, and $\boldsymbol{\sigma}_0 \in \mathcal{M}$ then $W_{\boldsymbol{n}}(\mathcal{M})$ must be convex and contain the origin. But $\mathcal{M}$ and hence $W_{\boldsymbol{n}}(\mathcal{M})$ have no interior, and a convex set with no interior must lie in a hyperplane. It follows that $W_{\boldsymbol{n}}(\mathcal{M})$ must lie in a hyperplane passing through the origin, i.e. in a subspace $\mathcal{K} = \mathcal{K}_{\boldsymbol{n}}$. Moreover, since $\mathcal{M}$ must be stable under lamination in all directions the set $W_{\boldsymbol{m}}(W_{\boldsymbol{n}}^{-1}(\mathcal{K}))$ must be a subspace for each choice of unit vector $\boldsymbol{m}$. Now given some tensor $\boldsymbol{K} \in \mathcal{K}$ and expanding $W_{\boldsymbol{m}}(W_{\boldsymbol{n}}^{-1}(\epsilon\boldsymbol{K}))$ in powers of ϵ gives

$$\begin{aligned} W_{\boldsymbol{m}}(W_{\boldsymbol{n}}^{-1}(\epsilon\boldsymbol{K})) &= \epsilon\boldsymbol{K}\{\boldsymbol{I} - [\boldsymbol{\Gamma}(\boldsymbol{n}) - \boldsymbol{\Gamma}(\boldsymbol{m})]\epsilon\boldsymbol{K}\}^{-1} \\ &= \epsilon\boldsymbol{K} + \epsilon^2\boldsymbol{K}\boldsymbol{A}(\boldsymbol{m})\boldsymbol{K} + \epsilon^3\boldsymbol{K}\boldsymbol{A}(\boldsymbol{m})\boldsymbol{K}\boldsymbol{A}(\boldsymbol{m})\boldsymbol{K} + \ldots, \end{aligned} \tag{19}$$

where $\boldsymbol{A}(\boldsymbol{m})$ is given by (18) with $\boldsymbol{M} = \boldsymbol{\Gamma}(\boldsymbol{n})$. Since the linear term is $\epsilon\boldsymbol{K}$ the hyperplane $W_{\boldsymbol{m}}(W_{\boldsymbol{n}}^{-1}(\mathcal{K}))$ must in fact be $\mathcal{K}$ itself, i.e. $\mathcal{K}$ does not depend on $\boldsymbol{n}$. From an examination of the quadratic term we then see that

$$\boldsymbol{K}\boldsymbol{A}(\boldsymbol{m})\boldsymbol{K} \in \mathcal{K} \quad \text{for all } \boldsymbol{m} \text{ and for all } \boldsymbol{K} \in \mathcal{K}. \tag{20}$$

Higher order terms in the expansion do not yield any additional constraints. Indeed substitution of $\boldsymbol{K}=\boldsymbol{K}_1+\boldsymbol{K}_2$ in (20), where $\boldsymbol{K}_1$ and $\boldsymbol{K}_2$ both lie in $\mathcal{K}$, yields the corollary,

$$\boldsymbol{K}_1\boldsymbol{A}(\boldsymbol{m})\boldsymbol{K}_2+\boldsymbol{K}_2\boldsymbol{A}(\boldsymbol{m})\boldsymbol{K}_1\in\mathcal{K} \quad \text{for all } \boldsymbol{K}_1,\boldsymbol{K}_2\in\mathcal{K}. \tag{21}$$

Applying this with $\boldsymbol{K}_1=\boldsymbol{K}$ and $\boldsymbol{K}_2=\boldsymbol{K}\boldsymbol{A}(\boldsymbol{m})\boldsymbol{K}$ shows that the cubic term lies in the space $\mathcal{K}$. Similarly all the remaining higher order terms must also lie in $\mathcal{K}$ once (20) is satisfied. Therefore the condition (20) is both necessary and sufficient to ensure the stability under lamination of the set of all conductivity tensors in $\mathcal{M}_c\cap W_{\boldsymbol{n}}^{-1}(\mathcal{K})$.

For example, consider two-dimensional conductivity and take $\boldsymbol{\sigma}_0=\sigma_0\boldsymbol{I}$. Then $\boldsymbol{A}(\boldsymbol{m})=(\boldsymbol{n}\otimes\boldsymbol{n}-\boldsymbol{m}\otimes\boldsymbol{m})/\sigma_0$ is a trace-free 2×2 symmetric matrix. Now trace free 2×2 symmetric matrices have the property that the product of any three such matrices is also trace free and symmetric. So (20) will be satisfied when $\mathcal{K}$ is the space of trace free 2×2 symmetric matrices. Then $W_{\boldsymbol{n}}^{-1}(\mathcal{K})$ consists of 2×2 symmetric matrices $\boldsymbol{\sigma}_*$ such that $\mathrm{Tr}[(\sigma_0\boldsymbol{I}-\boldsymbol{\sigma}_*)^{-1}]=1/\sigma_0$. Equivalently, it consists of matrices $\boldsymbol{\sigma}_*$ such that $\det\boldsymbol{\sigma}_*=\sigma_0^2$. This confirms that the manifold (11) is stable under lamination.

The preceeding analysis extends easily to the elasticity problem (and also to piezoelectric, thermoelectric, thermoelastic, pyroelectric and related coupled problems). Candidate exact relations are found by searching for subspaces $\mathcal{K}$ of fourth-order tensors $\mathcal{K}$ satisfying (20) where $\boldsymbol{A}(\boldsymbol{m})=\boldsymbol{\Gamma}(\boldsymbol{n})-\boldsymbol{\Gamma}(\boldsymbol{m})$ and $\boldsymbol{\Gamma}(\boldsymbol{k})$ is a fourth-order tensor dependent upon the choice of a reference elasticity tensor $\boldsymbol{\mathcal{C}}_0\in\mathcal{M}_e$. In particular, for three-dimensional elasticity, if $\boldsymbol{\mathcal{C}}_0$ is elastically isotropic with bulk modulus κ_0 and shear modulus μ_0, $\boldsymbol{\Gamma}(\boldsymbol{k})$ has cartesian elements

$$\begin{aligned}\{\boldsymbol{\Gamma}(\boldsymbol{k})\}_{ij\ell m} &= \frac{1}{4\mu_0}\Big(k_i\delta_{j\ell}k_m+k_i\delta_{jm}k_\ell+k_j\delta_{i\ell}k_m+k_j\delta_{im}k_\ell-4k_ik_jk_\ell k_m\Big)\\ &\quad+\frac{3k_ik_jk_\ell k_m}{3\kappa_0+4\mu_0}.\end{aligned} \tag{22}$$

Once such a subspace $\mathcal{K}$ is found the canditate exact relation is the set

$$\mathcal{M}=\mathcal{M}_e\cap W_{\boldsymbol{n}}^{-1}(\mathcal{K}), \tag{23}$$

where $W_{\boldsymbol{n}}^{-1}$ is the inverse of the transformation

$$W_{\boldsymbol{n}}(\boldsymbol{\mathcal{C}})=[\boldsymbol{\mathcal{I}}+(\boldsymbol{\mathcal{C}}-\boldsymbol{\mathcal{C}}_0)\boldsymbol{\Gamma}(\boldsymbol{n})]^{-1}(\boldsymbol{\mathcal{C}}-\boldsymbol{\mathcal{C}}_0). \tag{24}$$

Using a related procedure Grabovsky and Sage (1998) found as a canditate exact relation, stable under lamination, the manifold $\mathcal{M}=\mathcal{M}(\mu_0)$ consisting of all elasticity tensors in $\mathcal{M}_e$ expressible in the form

$$\boldsymbol{\mathcal{C}}=2\mu_0(\boldsymbol{\mathcal{I}}-\boldsymbol{I}\otimes\boldsymbol{I})+\boldsymbol{D}\otimes\boldsymbol{D}, \tag{25}$$

for some choice of symmetric second-order tensor $\boldsymbol{D}$, in which $\boldsymbol{\mathcal{I}}$ is the fourth-order identity tensor. We will establish that this manifold $\mathcal{M}$ does in fact define an exact relation valid for all composites and not just laminates. For planar elasticity the analogous exact relation was proved by Grabovsky and Milton (1998).

SUFFICIENT CONDITIONS FOR AN EXACT RELATION

We would like to show that the manifold $\mathcal{M}$ of elasticity tensors defined by (23) is stable under homogenization and not just lamination, i.e. to ensure that any composite with elasticity tensor $\boldsymbol{\mathcal{C}}(\boldsymbol{x}) \in \mathcal{M}$ always has an effective elasticity tensor $\boldsymbol{\mathcal{C}}_* \in \mathcal{M}$. Here we will prove it is sufficient that there exist a larger space of fourth-order tensors $\overline{\mathcal{K}}$ (not necessarily self-adjoint) such that

$$\boldsymbol{K}_1\boldsymbol{A}(\boldsymbol{m})\boldsymbol{K}_2 \in \overline{\mathcal{K}} \quad \text{for all } \boldsymbol{m} \text{ and for all } \boldsymbol{K}_1, \boldsymbol{K}_2 \in \overline{\mathcal{K}}, \tag{26}$$

and such that $\mathcal{K}$ equals the subspace of all self-adjoint tensors in $\overline{\mathcal{K}}$.

To avoid confusion let us first return to the setting of the conductivity problem. To find $\boldsymbol{K}_*$ and hence $\boldsymbol{\sigma}_*$ we need to solve (16) for a set of d different values $\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots \boldsymbol{v}_d$ of $\boldsymbol{v}$. Associated with each value $\boldsymbol{v}_i$ of $\boldsymbol{v}$ is a corresponding polarization field $\boldsymbol{p}_i(\boldsymbol{x})$. Let $\boldsymbol{V}$ and $\boldsymbol{P}(\boldsymbol{x})$ be the $d \times d$ matrices with the vectors $\boldsymbol{v}_i$ and $\boldsymbol{p}_i(\boldsymbol{x})$, $i = 1, 2, \ldots, d$, as columns. [Similar matrix valued fields were introduced by Murat and Tartar (1985).] Taking $\boldsymbol{V} = \boldsymbol{I}$ the set of equations (16) for $\boldsymbol{K}_*$ and the d polarization fields can be rewritten as

$$[\boldsymbol{I} - \boldsymbol{K}\boldsymbol{A}]\boldsymbol{P} = \boldsymbol{K}, \quad \langle \boldsymbol{P} \rangle = \boldsymbol{K}_*, \tag{27}$$

where now the field $\boldsymbol{Q} = \boldsymbol{K}\boldsymbol{A}\boldsymbol{P}$ is given by

$$\boldsymbol{Q}(\boldsymbol{x}) = \sum_{\boldsymbol{k} \neq 0} e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \boldsymbol{K}(\boldsymbol{x})\boldsymbol{A}(\boldsymbol{k})\widehat{\boldsymbol{P}}(\boldsymbol{k}), \tag{28}$$

in which $\widehat{\boldsymbol{P}}(\boldsymbol{k})$ is the Fourier component of $\boldsymbol{P}(\boldsymbol{x})$, and $\boldsymbol{K}(\boldsymbol{x})\boldsymbol{A}(\boldsymbol{k})$ acts on $\widehat{\boldsymbol{P}}(\boldsymbol{k})$ by matrix multiplication. The extension of this analysis to elasticity is mathematically straight-forward, but physically intriguing since in the elasticity setting $\boldsymbol{P}(\boldsymbol{x})$ is taken as a fourth-order tensor field.

Provided $\boldsymbol{K}(\boldsymbol{x})$ is sufficiently small for all $\boldsymbol{x}$, i.e. $\boldsymbol{\sigma}(\boldsymbol{x})$ is close to $\boldsymbol{\sigma}_0$, the solution to (27) is given by the perturbation expansion

$$\boldsymbol{P}(\boldsymbol{x}) = \sum_{j=0}^{\infty} \boldsymbol{P}_j(\boldsymbol{x}) \quad \text{where } \boldsymbol{P}_j = (\boldsymbol{K}\boldsymbol{A})^j \boldsymbol{K}. \tag{29}$$

Now let us suppose $\boldsymbol{K}(\boldsymbol{x})$ takes values in a tensor subspace $\overline{\mathcal{K}}$ satisfying (26). Our objective is to prove that each field $\boldsymbol{P}_j(\boldsymbol{x})$ in the perturbation expansion also takes values in $\overline{\mathcal{K}}$. Certainly the first term $\boldsymbol{P}_0(\boldsymbol{x}) = \boldsymbol{K}(\boldsymbol{x})$ does. Also if for some $j \geq 0$ the field $\boldsymbol{P}_j$ takes values in $\overline{\mathcal{K}}$ then its Fourier coefficients also take values in $\overline{\mathcal{K}}$ and (28) together with (26) implies that $\boldsymbol{P}_{j+1} = \boldsymbol{K}\boldsymbol{A}\boldsymbol{P}_j$ also lies in $\overline{\mathcal{K}}$. By induction it follows that every term in the expansion takes values in $\overline{\mathcal{K}}$. Provided the perturbation expansion converges this implies that $\langle \boldsymbol{P} \rangle = \boldsymbol{K}_*$ lies in $\overline{\mathcal{K}}$. Even if the perturbation expansion does not converge, analytic continuation arguments imply the exact relation still holds provided $\boldsymbol{\sigma}(\boldsymbol{x}) \in \mathcal{M}_c$ for all $\boldsymbol{x}$, as will be shown in a forthcoming paper.

The effective shear modulus of a family of polycrystals

To illustrate the power of this method of generating exact relations, let us consider three-dimensional elasticity and prove that the manifold $\mathcal{M}$ consisting of all elasticity tensors in $\mathcal{M}_e$ expressible in the form (25) for some choice of $\boldsymbol{D}$ defines an exact relation. We take $\boldsymbol{\mathcal{C}}_0$ to be an arbitrary isotropic elastcity tensor with bulk modulus κ_0 and shear modulus μ_0. The associated tensor $\boldsymbol{\Gamma}(\boldsymbol{n})$, given by (22) has the property that $\mathrm{Tr}[\boldsymbol{\Gamma}(\boldsymbol{m})\boldsymbol{I}]$ is independent of $\boldsymbol{m}$ implying that with

$$\boldsymbol{M} = \boldsymbol{I}\otimes\boldsymbol{I}/3(3\kappa_0+4\mu_0), \tag{30}$$

we have

$$\mathrm{Tr}\{[\boldsymbol{M}-\boldsymbol{\Gamma}(\boldsymbol{m})]\boldsymbol{I}\} = 0 \quad \text{for all } \boldsymbol{m}. \tag{31}$$

Now consider the subspace $\overline{\mathcal{K}}$ consisting of all fourth order tensors $\boldsymbol{K}$ expressible in the form $\boldsymbol{K} = \boldsymbol{I}\otimes\boldsymbol{B}+\boldsymbol{B}'\otimes\boldsymbol{I}$ for some choice of symmetric matrices $\boldsymbol{B}$ and $\boldsymbol{B}'$. Now given symmetric matrices $\boldsymbol{B}_1$, $\boldsymbol{B}_1'$, $\boldsymbol{B}_2$ and $\boldsymbol{B}_2'$ (31) implies there exist symmetric matrices $\boldsymbol{B}_3$ and $\boldsymbol{B}_3'$ such that

$$[\boldsymbol{I}\otimes\boldsymbol{B}_1+\boldsymbol{B}_1'\otimes\boldsymbol{I}]\boldsymbol{A}(\boldsymbol{m})[\boldsymbol{I}\otimes\boldsymbol{B}_2+\boldsymbol{B}_2'\otimes\boldsymbol{I}] = \boldsymbol{I}\otimes\boldsymbol{B}_3+\boldsymbol{B}_3'\otimes\boldsymbol{I}. \tag{32}$$

Therefore the subspace $\overline{\mathcal{K}}$ satisfies the desired property (26). The subspace $\mathcal{K}$ of self-adjoint fourth-order tensors within $\overline{\mathcal{K}}$ is six-dimensional consisting of all tensors of the form $\boldsymbol{K} = \boldsymbol{I}\otimes\boldsymbol{B}+\boldsymbol{B}\otimes\boldsymbol{I}$, where $\boldsymbol{B}$ is a symmetric matrix. When $\boldsymbol{K} = \boldsymbol{I}\otimes\boldsymbol{B}+\boldsymbol{B}\otimes\boldsymbol{I}$ and $3\kappa_0+4\mu_0-2\mathrm{Tr}\boldsymbol{B} > 0$ algebraic manipulation shows that

$$\boldsymbol{\mathcal{C}} = W_{\boldsymbol{M}}^{-1}(\boldsymbol{K}) = 2\mu_0(\boldsymbol{\mathcal{I}}-\boldsymbol{I}\otimes\boldsymbol{I})+\boldsymbol{D}\otimes\boldsymbol{D}, \tag{33}$$

with

$$\boldsymbol{D} = [3\kappa_0+4\mu_0-\mathrm{Tr}\boldsymbol{B})\boldsymbol{I}+3\boldsymbol{B}]/\sqrt{3(3\kappa_0+4\mu_0-2\mathrm{Tr}\boldsymbol{B})}. \tag{34}$$

The manifold $\mathcal{M}$ associated with $\mathcal{K}$ therefore consists of all tensors $\boldsymbol{\mathcal{C}} \in \mathcal{M}_e$ expressible in the form (25), and is stable under homogenization.

As an example, consider a three-dimensional elastic polycrystal where the elasticity tensor takes the form

$$\boldsymbol{\mathcal{C}}(\boldsymbol{x}) = \boldsymbol{R}(\boldsymbol{x})\boldsymbol{R}(\boldsymbol{x})\boldsymbol{\mathcal{C}}_0\boldsymbol{R}^T(\boldsymbol{x})\boldsymbol{R}^T(\boldsymbol{x}), \tag{35}$$

where $\boldsymbol{R}(\boldsymbol{x})$ is a rotation matrix, giving the orientation of the crystal at each point $\boldsymbol{x}$ and $\boldsymbol{\mathcal{C}}_0$ is the elasticity tensor of a single crystal which we assume has the form

$$\boldsymbol{\mathcal{C}}_0 = 2\mu_0(\boldsymbol{\mathcal{I}}-\boldsymbol{I}\otimes\boldsymbol{I})+\boldsymbol{D}_0\otimes\boldsymbol{D}_0, \quad \text{where} \quad [\mathrm{Tr}(\boldsymbol{D}_0)]^2-2\mathrm{Tr}(\boldsymbol{D}_0^2) > 4\mu_0 > 0, \tag{36}$$

in which the latter condition ensures that $\boldsymbol{\mathcal{C}}_0$ is positive definite. The elasticity tensor field $\boldsymbol{\mathcal{C}}(\boldsymbol{x})$ is of the required form (25) with $\boldsymbol{D}(\boldsymbol{x}) = \boldsymbol{R}(\boldsymbol{x})\boldsymbol{D}_0\boldsymbol{R}^T(\boldsymbol{x})$ and therefore the effective tensor $\boldsymbol{\mathcal{C}}_*$ of the polycrystal must lie on the manifold $\mathcal{M}$ for some $\beta > \alpha > 0$. In particular if $\boldsymbol{\mathcal{C}}_*$ is isotropic then its shear modulus is μ_0, independent of the polycrystal microgeometry. For planar elasticity the analogous result was proved by Avellaneda et. al. (1996).

Some interesting exact relations for coupled field problems

We are left with the algebraic problem of characterizing which tensor subspaces satisfy the conditions (20) or (26). One might wonder if there is perhaps some easy characterization. For elasticity and conductivity in two or three dimensions all possible rotationally invariant exact relations have now been found [see Grabovsky (1998), Grabovsky and Sage (1988) and references therein] but in a more general context the following example shows that the task is not so simple.

Consider a coupled field problem where there are there are m divergence free fields $\boldsymbol{j}_1(\boldsymbol{x}), \boldsymbol{j}_2(\boldsymbol{x}), ..., \boldsymbol{j}_m(\boldsymbol{x})$ and m curl free fields $\boldsymbol{e}_1(\boldsymbol{x}), \boldsymbol{e}_2(\boldsymbol{x}), ..., \boldsymbol{e}_m(\boldsymbol{x})$ which are linked through the constitutive relation

$$j_{i\alpha}(\boldsymbol{x}) = \sum_{j=1}^{d} \sum_{\beta=1}^{m} L_{i\alpha j\beta}(\boldsymbol{x}) e_{j\beta}(\boldsymbol{x}), \tag{37}$$

where α and β are field indices while i and j are space indices. Milgrom and Shtrikman (1989) have obtained some very useful exact relations for coupled field problems. Rather than rederiving these let us look for exact relations with $\boldsymbol{M} = 0$ and a reference tensor $\boldsymbol{L}_0$ which is the identity tensor $\boldsymbol{I}$. The associated tensor $\boldsymbol{A}(\boldsymbol{m}) = \boldsymbol{M} - \boldsymbol{\Gamma}(\boldsymbol{m})$ has elements $A_{i\alpha j\beta} = -\delta_{\alpha\beta} m_i m_j$. Now take $\mathcal{R}$ to be a r-dimensional subspace of $m \times m$ matrices and let $\mathcal{S}$ denote the d^2-dimensional space of $d \times d$ matrices, and consider the rd^2-dimensional subspace $\overline{\mathcal{K}}$ spanned by all tensors $\boldsymbol{K}$ which are tensor products of matrices $\boldsymbol{R} \in \mathcal{R}$ and matrices $\boldsymbol{S} \in \mathcal{S}$, i.e. which have elements $K_{i\alpha j\beta} = R_{\alpha\beta} S_{ij}$. Given a tensor $\boldsymbol{K}_1$ which is the tensor product of $\boldsymbol{R}_1 \in \mathcal{R}$ and $\boldsymbol{S}_1 \in \mathcal{S}$ and a tensor $\boldsymbol{K}_2$ which is the tensor product of $\boldsymbol{R}_2 \in \mathcal{R}$ and $\boldsymbol{S}_2 \in \mathcal{S}$, the product $\boldsymbol{K}_1 \boldsymbol{A}(\boldsymbol{m}) \boldsymbol{K}_2$ will certainly be in $\overline{\mathcal{K}}$ provided $\boldsymbol{R}_1 \boldsymbol{R}_2 \in \mathcal{R}$. Moreover if this holds for all $\boldsymbol{R}_1, \boldsymbol{R}_2 \in \mathcal{R}$ then $\overline{\mathcal{K}}$ defines an exact relation because it is spanned by matrices of the same form as $\boldsymbol{K}_1$ and $\boldsymbol{K}_2$. This observation allows us to generate countless exact relations. The condition on $\mathcal{R}$ just says that it is closed under multiplication, i.e. that it forms an algebra. Unfortunately there is no known way of characterizing which subspaces of matrices form an algebra for general m, and this hints of the difficulties involved in trying to obtain a complete characterization of exact relations. Since $\boldsymbol{M} = 0$ the manifold $\mathcal{M}$ consists of an appropriately bounded coercive subset of tensors of the form $\boldsymbol{L} = \boldsymbol{I} + \boldsymbol{K}$ where $\boldsymbol{K} \in \overline{\mathcal{K}}$. The case where $m = 2$ and $\mathcal{R}$ is the set of all 2×2 matrices of the form $\boldsymbol{R} = a\boldsymbol{I} + b\boldsymbol{R}_\perp$ (which is clearly closed under multiplication) corresponds to tensor fields $\boldsymbol{L}(\boldsymbol{x})$ for which the consitutive relation can be rewritten in the equivalent form of a complex equation

$$\boldsymbol{j}_1(\boldsymbol{x}) + i\boldsymbol{j}_2(\boldsymbol{x}) = (\boldsymbol{A}(\boldsymbol{x}) + i\boldsymbol{B}(\boldsymbol{x}))(\boldsymbol{e}_1(\boldsymbol{x}) + i\boldsymbol{e}_2(\boldsymbol{x})). \tag{38}$$

The effective tensor $\boldsymbol{L}_*$ will have an associated complex form $\boldsymbol{A}_* + i\boldsymbol{B}_*$.

References

Avellaneda, M., Cherkaev, A.V., Gibiansky, L.V., Milton, G.W., and Rudelson, M. 1996 *J. Mech. Phys. Solids* 44, 1179-1218.

Backus, G.E. 1962 *J. Geophys. Res.* 67, 4427-4440.

Bensoussan, A., Lions, J.L., and Papanicolaou, G. 1978 *Asymptotic analysis for periodic structures. Studies in mathematics and its applications*, 5, North-Holand.

Dvorak, G.J., and Benveniste, Y. 1997 In *Theoretical and Applied Mechanics 1996*, pp. 217-237, ed. by T.Tatsumi, E.Watanabe, and T.Kambe, Elsevier.

Dykhne, A.M. 1970 *Zh. Eksp. Teor. Fiz.* 59 , 110-115. [*Soviet Physics JETP* 32 (1971), 63-65.]

Grabovsky, Y., and Milton, G.W. 1998 *Proc. Roy. Soc. Edin. A* 128, 283-299.

Grabovsky, Y., 1998 *Arch. Rat. Mech. Anal.* to appear.

Grabovsky, Y., and Sage, D.S. 1998 *Arch. Rat. Mech. Anal.* to appear.

Hill, R. 1952 *Proc. Phys. Soc. Lond. A* 65, 349-354.

Keller, J.B. 1964 *J. Math. Phys.* 5, 548-549.

Lurie, K.A., and Cherkaev, A.V. 1981 *Dokl. Akad. Nauk.* 259, 328-331.

Lurie, K.A., Cherkaev, A.V., and Fedorov, A.V. 1984 *J. Opt. Theory Appl.* 42, 247-281.

Mendelson, K.S. 1975 *J. Appl. Phys.* 46, 4740-4741.

Milgrom, M. and Shtrikman, S. 1989 *Phys. Rev. A* 40, 1568-1575.

Milton, G.W. 1997 In *Theoretical and Applied Mechanics 1996*, pp. 443-459, ed. by T.Tatsumi, E.Watanabe, and T.Kambe, Elsevier.

Murat, F. and Tartar, L. 1985 In *Les méthodes de l'homogénéisation: théorie et applications en physique, Coll. de la Dir. des Études et Recherches de Électricité de France*, Eyrolles, Paris, 319-370.

Murat, F., and Tartar, L. 1997 In *Topics in the mathematical modelling of composite materials*, ed. by A. Cherkaev and R. Kohn, *Progress in nonlinear differential equations and their applications*, 31, pp. 21-43, Birkhauser.

Tartar, L. 1976 In *Computer Methods in Applied Sciences and Engineering*, R. Glowinski, J.-L. Lions eds., Springer-Verlag Lecture Notes in Mathematics 704, pp.136-212, Springer-Verlag.

Zhikov (Jikov), V.V., Kozlov, S.M., and Oleinik, O.A. 1994 *Homogenization of differential operators and integral functionals*, Springer-Verlag.

Yury Grabovsky
Department of Mathematics
The University of Utah
Salt Lake City, Utah 84112, U.S.A.
yuri@math.utah.edu

Graeme W. Milton
Department of Mathematics
The University of Utah
Salt Lake City, Utah 84112, U.S.A.
milton@math.utah.edu