

Review



Cite this article: Milton GW. 2021 Some open problems in the theory of composites. *Phil. Trans. R. Soc. A* **379**: 20200115.
<https://doi.org/10.1098/rsta.2020.0115>

Accepted: 16 November 2020

One contribution of 10 to a theme issue 'Topics in mathematical design of complex materials'.

Subject Areas:

applied mathematics, differential equations, mechanical engineering, materials science

Keywords:

composites, effective moduli, quasi-convexity, homogenization, bounds, laminates

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Some open problems in the theory of composites

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A selection of open problems in the theory of composites is presented. Particular attention is drawn to the question of whether two-dimensional, two-phase composites with general geometries have the same set of possible effective tensors as those of hierarchical laminates. Other questions involve the conductivity and elasticity of composites. Finally, some future directions for wave and other equations are mentioned.

This article is part of the theme issue 'Topics in mathematical design of complex materials'.

1. Introduction

The theory of composite materials has seen a resurgence of interest thanks to the discovery of novel properties and a dramatic rise in our ability to manufacture desired microgeometries: see, for instance, the review [1] and references therein. Back in the 1980s and 1990s, there was also a rapid increase in interest, partly due to the recognition that the solution of optimal design problems often requires composite microstructures in the design. This gave rise to the area of topology optimization which has had enormous impact, moving into the mainstream of engineering design: see, for example, the book [2]. From a mathematics perspective there were accompanying rapid developments: in our understanding of homogenization, which underlies the use of effective moduli to describe macroscopic responses; in bounds on effective moduli, coupled with the identification of microstructures that attain them; in the theory governing microgeometry independent exact relations satisfied by effective moduli; and in the discovery of composites with unexpected properties, as surveyed in the books [3–11].

Given the recent interest, it is perhaps appropriate to draw attention to some of the open problems generated in the mathematical research that is now mostly over three decades old, as well as questions generated by more recent investigations. The problems here are by no means exhaustive. Rather, they are ones I have encountered in my research work and found quite difficult, usually because I have no idea how to solve them. Some are just of theoretical interest, while others should be of interest to both experimentalists and theorists alike. The problems reflect my own research interests, both past and present, and other experts in the field would undoubtedly choose a different set. Many are old outstanding problems, where it is difficult to dig in the hard soil, but some address new topics where the soil is more fertile and it is easier to break ground.

2. Open problems involving quasi-convexification

Here we present a selection of open problems that are related to quasi-convexification. For a recent survey of selected results pertaining to quasi-convexity, and the closely related topic of weak lower semicontinuity, see [12,13] and references therein. The focus is largely on two-phase composites, and the corresponding two-well quasi-convexification problems, since these are perhaps of greatest interest in the field of composites (though some effects, such as getting negative or unbounded thermal expansion coefficients from materials having only positive thermal expansion coefficients, require at least three phases [14,15]). In this age of 3D-printing, it is now relatively easy to manufacture tailored microstructures of one phase plus void that can then be infilled to obtain a two-phase material. One is interested in the range the effective tensors can have as the microgeometry varies over all configurations. This range is known as the G -closure and provides limits for what one can expect to achieve when one tries to optimize the local response using relatively simple practical microstructures obtained, for example, by topology optimization. The question we explore is whether it suffices to consider only hierarchical laminate geometries rather all conceivable microstructures. Hierarchical laminate geometries have the advantage that it is relatively easy to calculate their effective properties (for example [16,17], ch. 9 in [7] and references therein).

We start with:

Problem 2.1. Is rank-one convexity equal to quasi-convexity for the two-well problem in two spatial dimensions?

Given two self-adjoint positive definite mappings \mathbf{L}_1 and \mathbf{L}_2 on the space \mathcal{S}_m of real $2 \times m$ matrices, equipped with the standard inner product

$$\mathbf{A}_1 \cdot \mathbf{A}_2 = \text{Tr}(\mathbf{A}_1 \mathbf{A}_2^T), \quad (2.1)$$

where Tr denotes the trace, and $\mathbf{A}_1, \mathbf{A}_2 \in \mathcal{S}_m$, and given $\mathbf{F}_1, \mathbf{F}_2 \in \mathcal{S}_m$, and two reals c_1 and c_2 , consider the two well ‘energy’,

$$W(\mathbf{F}) = \min\{W_1(\mathbf{F}), W_2(\mathbf{F})\}, \quad \mathbf{F} \in \mathcal{S}_m, \quad (2.2)$$

where the $W_j(\mathbf{F})$, $j = 1, 2$, are the quadratic wells

$$\begin{aligned} W_j(\mathbf{F}) &= (\mathbf{F} - \mathbf{F}_j) \cdot \mathbf{L}_j(\mathbf{F} - \mathbf{F}_j) + k_j \\ &= \mathbf{F} \cdot \mathbf{L}_j \mathbf{F} + 2\mathbf{V}_j \cdot \mathbf{F} + c_j, \quad \mathbf{V}_j = -\mathbf{L}_j \mathbf{F}_j, \quad c_j = k_j + \mathbf{F}_j \cdot \mathbf{L}_j \mathbf{F}_j. \end{aligned} \quad (2.3)$$

The quasi-convexification of $W(\mathbf{F})$ is given by

$$QW(\mathbf{F}) = \inf_{\mathbf{u}} (W(\mathbf{F} + \nabla \mathbf{u})), \quad (2.4)$$

where the infimum is over all m -component periodic potentials $\mathbf{u}(\mathbf{x})$ and the average $\langle \cdot \rangle$ is over the unit cell of periodicity. (We adopt the convention that the elements of $\nabla \mathbf{u}$ are $\{\nabla \mathbf{u}\}_{ij} = \partial u_j / \partial x_i$.)

An energy $W_0(\mathbf{F})$ is said to be rank-one convex if

$$W_0(\mathbf{a} \otimes \mathbf{b}) \leq pW_0(\mathbf{a} \otimes \mathbf{b}) + (1-p)W_0(\mathbf{a} \otimes \mathbf{b}), \quad (2.5)$$

for all real $p \in [0, 1]$, all real 2-component vectors \mathbf{a} , and all real m -component vectors \mathbf{b} . The rank-one convexification of $W(\mathbf{F})$, denoted $RW(\mathbf{F})$, is the highest rank-one convex energy that lies equal or below $W(\mathbf{F})$ for all \mathbf{F} . So the question is whether $QW(\mathbf{F}) = RW(\mathbf{F})$ for all choices of m , \mathbf{K}_1 , \mathbf{K}_2 , \mathbf{F}_1 , \mathbf{F}_2 , c_1 , c_2 ? We will see that this can be reduced to the problem with $\mathbf{F}_1 = \mathbf{F}_2 = 0$. Clearly, the problem does not change if we add the same constant to c_1 and c_2 . So without loss of generality we can assume that c_1 and c_2 are sufficiently large so that

$$\mathbf{K}_1 = \begin{pmatrix} \mathbf{L}_1 & \mathbf{V}_1 \\ \mathbf{V}_1^T & c_1 \end{pmatrix} > 0, \quad \mathbf{K}_2 = \begin{pmatrix} \mathbf{L}_2 & \mathbf{V}_2 \\ \mathbf{V}_2^T & c_2 \end{pmatrix} > 0. \quad (2.6)$$

In terms of these, we have

$$W_j(\mathbf{F}) = \begin{pmatrix} \mathbf{F} \\ 1 \end{pmatrix} \cdot \mathbf{K}_j \begin{pmatrix} \mathbf{F} \\ 1 \end{pmatrix}, \quad (2.7)$$

in which the inner product is the obvious generalization of (2.1).

In the field of composites problem 2.1 is equivalent to the following question:

Problem 2.2. For two-phase composites in two spatial dimensions, such that phase 1 occupies a volume fraction f , is the G_f -closure equal to its lamination closure when the fields on the right of the constitutive law have n components, each being the sum of a real 2 component vector and the gradient of a scalar periodic potential, while the fields on the left of the constitutive law also have n components, each having zero divergence, in which n is an arbitrary positive integer?

The constitutive law takes the form

$$\underbrace{\begin{pmatrix} \mathbf{j}^{(1)}(\mathbf{x}) \\ \mathbf{j}^{(2)}(\mathbf{x}) \\ \vdots \\ \mathbf{j}^{(k)}(\mathbf{x}) \end{pmatrix}}_{\mathbf{J}(\mathbf{x})} = \mathbf{L}(\mathbf{x}) \underbrace{\begin{pmatrix} \mathbf{e}^{(1)}(\mathbf{x}) \\ \mathbf{e}^{(2)}(\mathbf{x}) \\ \vdots \\ \mathbf{e}^{(k)}(\mathbf{x}) \end{pmatrix}}_{\mathbf{E}(\mathbf{x})}, \quad (2.8)$$

where the $\mathbf{j}^{(i)}(\mathbf{x})$, $\mathbf{e}^{(j)}(\mathbf{x})$, $\mathbf{L}(\mathbf{x})$ all have the same periodicity and satisfy

$$\nabla \cdot \mathbf{j}^{(i)} = 0, \quad \mathbf{e}^{(j)} = \mathbf{e}_0^{(j)} + \nabla V_j, \quad \mathbf{L}(\mathbf{x}) = \chi(\mathbf{x})\mathbf{L}_1 + [1 - \chi(\mathbf{x})]\mathbf{L}_2, \quad (2.9)$$

in which the $\mathbf{e}_0^{(j)}$ are constant vectors, the $V_j(\mathbf{x})$ are periodic potentials, $\chi(\mathbf{x})$ is the indicator function

$$\begin{aligned} \chi(\mathbf{x}) &= 1 && \text{in phase 1,} \\ &= 0 && \text{in phase 2,} \end{aligned} \quad (2.10)$$

satisfying $\langle \chi \rangle = f$, in which the angular brackets $\langle \cdot \rangle$ denote a volume average over the unit cell of periodicity, and \mathbf{L}_1 and \mathbf{L}_2 are self-adjoint positive definite mappings on \mathcal{S}_n . Thus \mathbf{L}_1 and \mathbf{L}_2 take the block matrix form

$$\mathbf{L}_j = \begin{pmatrix} \sigma_j^{(11)} & \sigma_j^{(12)} & \cdots & \sigma_j^{(1n)} \\ \sigma_j^{(21)} & \sigma_j^{(22)} & \cdots & \sigma_j^{(2n)} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_j^{(n1)} & \sigma_j^{(n2)} & \cdots & \sigma_j^{(nn)} \end{pmatrix}, \quad j = 1, 2, \quad (2.11)$$

in which each $\sigma_j^{(k\ell)}$ is a 2×2 matrix, with $\sigma_j^{(k\ell)} = [\sigma_j^{(\ell k)}]^T$. The linear relation

$$\langle \mathbf{J} \rangle = \mathbf{L}_* \langle \mathbf{E} \rangle \quad (2.12)$$

determines the effective tensor \mathbf{L}_* . The G_f -closure, $G_f(\mathbf{L}_1, \mathbf{L}_2)$, is the closure of the set of values \mathbf{L}_* takes as $\chi(\mathbf{x})$ ranges over all possible indicator functions satisfying $\langle \chi \rangle = f$. In other words, the microstructure varies over all possible configurations in which phase 1 occupies a volume fraction f . The lamination closure, $G^L(\mathbf{L}_1, \mathbf{L}_2)$ is the closure of the set of values \mathbf{L}_* takes as $\chi(\mathbf{x})$ ranges over the indicator functions of multiple-rank laminate materials satisfying $\langle \chi \rangle = f$. Multiple-rank laminate materials are hierarchical materials, obtained by an iterative process of lamination in different directions on larger and larger length scales, ideally with an infinite ratio between the length scales at each stage of construction. A rank-one laminate is just a simple laminate of the phases, which can be regarded as rank-zero laminates. A rank m laminate is obtained by layering together a rank $m-1$ laminate with a laminate of rank $m-1$ or less.

The G -closure, $G(\mathbf{L}_1, \mathbf{L}_2)$, is the closure of the set of values \mathbf{L}_* takes as $\chi(\mathbf{x})$ ranges over all possible indicator functions, while the associated lamination closure $G^L(\mathbf{L}_1, \mathbf{L}_2)$ is the closure of the set of values \mathbf{L}_* takes as $\chi(\mathbf{x})$ ranges over the indicator functions of multiple-rank laminate materials. These are the union over $f \in [0, 1]$ of $G_f(\mathbf{L}_1, \mathbf{L}_2)$ and $G_f^L(\mathbf{L}_1, \mathbf{L}_2)$, respectively.

Remark 2.3. The equivalence of $G_f(\mathbf{L}_1, \mathbf{L}_2)$ and $G_f^L(\mathbf{L}_1, \mathbf{L}_2)$ in the case $n = 1$ has been established by Nesi [18] and Grabovsky [19,20], subject to certain assumptions about $\mathbf{L}_1 = \sigma_1^{(11)}$ and $\mathbf{L}_2 = \sigma_2^{(11)}$. (The $n = 1$ case where \mathbf{L}_1 and \mathbf{L}_2 do not commute, and $\mathbf{L}_1 - \mathbf{L}_2$ is neither positive nor negative semidefinite, is unresolved to my knowledge). They built on earlier work of Lurie & Cherkaev [21] and Murat & Tartar [22], who treated, using a variational approach known as the translation method, or method of compensated compactness, the case where $\sigma_1^{(11)}$ and $\sigma_2^{(11)}$ are both proportional to the identity matrix, corresponding to isotropic materials. For $n = 2$, it is an open question as to whether they are equivalent. In planar elasticity with two, possibly anisotropic, phases with fixed orientations, which is a subcase of the $n = 2$ case, existing evidence points to them being equivalent. In three-dimensional elasticity, one needs microstructures, such as pentamode materials [23], that are stiff with respect to one loading, yet compliant with respect to all other loadings (which span a five-dimensional space), and it is by no means clear that their behaviour can be mimicked by hierarchical laminate structures.

Remark 2.4. In two spatial dimensions, Grabovsky [24] has an example of a manifold \mathcal{M} of tensors \mathbf{L} that is stable under lamination but not under homogenization. This suggests that by picking anisotropic $\mathbf{L}_1, \mathbf{L}_2 \in \mathcal{M}$ one might find a $\chi(\mathbf{x})$ such that \mathbf{L}_* is not in \mathcal{M} , thus establishing that $G(\mathbf{L}_1, \mathbf{L}_2)$ and $G^L(\mathbf{L}_1, \mathbf{L}_2)$ differ. However, the analysis showing that \mathcal{M} is stable under lamination [25] extends directly to all two-phase composite geometries as can be seen from [26] once one takes the ‘reference tensor’ \mathbf{L}_0 equal to \mathbf{L}_2 . We conclude that $\mathbf{L}_* \in \mathcal{M}$. The same analysis applies to any manifold \mathcal{M} stable under lamination in any spatial dimension: if $\mathbf{L}_1, \mathbf{L}_2 \in \mathcal{M}$ then also $\mathbf{L}_* \in \mathcal{M}$, for any indicator function $\chi(\mathbf{x})$, not just those corresponding to laminate geometries.

Remark 2.5. If indeed $G(\mathbf{L}_1, \mathbf{L}_2)$ and $G^L(\mathbf{L}_1, \mathbf{L}_2)$ differ for some n and some $\mathbf{L}_1 \geq 0$ and $\mathbf{L}_2 \geq 0$, the next questions become: can one identify the minimum value n_0 of n for which they differ for some \mathbf{L}_1 and \mathbf{L}_2 , and given $n \geq n_0$ can one identify the set of pairs $(\mathbf{L}_1, \mathbf{L}_2)$ for which they differ, or for which $G_f(\mathbf{L}_1, \mathbf{L}_2)$ and $G_f^L(\mathbf{L}_1, \mathbf{L}_2)$ differ for fixed f ? More generally, if one has a composite with k phases, what is the smallest value of n for which $G(\mathbf{L}_1, \mathbf{L}_2, \dots, \mathbf{L}_k)$ and $G^L(\mathbf{L}_1, \mathbf{L}_2, \dots, \mathbf{L}_k)$ differ, or for which $G(\mathbf{K}_1, \mathbf{K}_2, \dots, \mathbf{K}_k)$ and $G^L(\mathbf{K}_1, \mathbf{K}_2, \dots, \mathbf{K}_k)$ differ, where the \mathbf{K}_j are defined analogously to (2.6)? A variant of an example of Šverák [27] shows that $G(\mathbf{K}_1, \mathbf{K}_2, \dots, \mathbf{K}_7)$ and $G^L(\mathbf{K}_1, \mathbf{K}_2, \dots, \mathbf{K}_7)$ differ when $n = 3$ (see section 31.9 of [7]).

Remark 2.6. In three spatial dimensions, it seems quite likely that there are two-phase geometries such that $G(\mathbf{L}_1, \mathbf{L}_2)$ and $G^L(\mathbf{L}_1, \mathbf{L}_2)$ differ. To obtain a candidate example, one considers the conductivity equations in the presence of a small magnetic field $\mathbf{h} = (h_1, h_2, h_3)$. In a two-phase

medium where phase 1 is isotropic while phase 2 is void, these take the form

$$\mathbf{j}(\mathbf{x}) = \chi(\mathbf{x})\boldsymbol{\rho}^{-1}\mathbf{e}(\mathbf{x}), \quad \nabla \cdot \mathbf{j} = 0, \quad \mathbf{e} = \mathbf{e}_0 + \nabla V, \quad \boldsymbol{\rho} = \boldsymbol{\rho}\mathbf{I} + R^H \begin{pmatrix} 0 & -h_3 & h_2 \\ h_3 & 0 & -h_1 \\ -h_2 & h_1 & 0 \end{pmatrix}, \quad (2.13)$$

where R^H is the Hall coefficient of phase 1, and $\boldsymbol{\rho}$ is its resistivity tensor. Assuming that the microstructure is isotropic or has cubic symmetry, the effective resistivity tensor $\boldsymbol{\rho}_* = \boldsymbol{\sigma}_*^{-1}$ (if it exists) to first order in \mathbf{h} takes the form

$$\boldsymbol{\rho}_* = \boldsymbol{\rho}_*\mathbf{I} + R_*^H \begin{pmatrix} 0 & -h_3 & h_2 \\ h_3 & 0 & -h_1 \\ -h_2 & h_1 & 0 \end{pmatrix}. \quad (2.14)$$

Numerical results [28,29] and corresponding physical experiments [30] show that in certain microstructures of interlinked tori, arranged to have cubic symmetry, R_*^H and R^H can have opposite signs. While it was commonly believed that the sign of Hall coefficient corresponds to the sign of the charge carrier, these composites provide a counterexample as they show the macroscopic Hall coefficient can be opposite in sign to the Hall coefficients of the constituent materials, assuming their Hall coefficients are zero or share a common sign. The argument that the Hall coefficient corresponds to the sign of the charge carrier assumes that the electrons, or holes, travel in straight lines, which of course is not the case in these composite materials. The microstructures were motivated by a three-phase example [31] having cubic symmetry, where it was rigorously shown that the Hall coefficients R_1^H, R_2^H and R_3^H of all three isotropic phases can be non-negative, while at the same time R_*^H is negative. One can explain this [29,31] in terms of the 'matrix valued' electric field $\mathbf{E}(\mathbf{x})$ whose three column vectors $\mathbf{e}_1(\mathbf{x}), \mathbf{e}_2(\mathbf{x})$, and $\mathbf{e}_3(\mathbf{x})$ each solve the conductivity equations, with zero magnetic field (i.e. the same $\chi(\mathbf{x})$ and $\boldsymbol{\rho} = \boldsymbol{\rho}\mathbf{I}$). Assuming $\langle \mathbf{E} \rangle = \mathbf{I}$, a perturbation argument [31,32] shows that the sign change of the Hall coefficient is related to the fact that the trace of the cofactor matrix of $\mathbf{E}(\mathbf{x})$ changes sign, at least in certain regions in the unit cell of periodicity. On the other hand, in any multiple rank laminates (with $\langle \mathbf{E} \rangle = \mathbf{I}$) Briane and Nesi show that the determinant of $\mathbf{E}(\mathbf{x})$ remains positive [33], whereas it does take negative values in certain regions in the interlinked tori geometries [34]. While they show that the trace of the cofactor matrix of $\mathbf{E}(\mathbf{x})$ can change sign in three-phase multiple rank laminates, it is an open question as to whether it can change sign in two-phase multiple rank laminates. If it cannot, then the path is clear to establishing that there are three-dimensional two-phase geometries such that $G(\mathbf{L}_1, \mathbf{L}_2)$ and $G^L(\mathbf{L}_1, \mathbf{L}_2)$ differ. We add that while in (2.13) the conductivity tensor $\boldsymbol{\sigma}(\mathbf{x}) = \chi(\mathbf{x})\boldsymbol{\rho}^{-1}$ is not symmetric, one can perturb the problem slightly so that phase 2 is slightly conducting, and then, using ideas of Cherkaev & Gibiansky [35], make a transformation to an equivalent problem where the tensor entering the constitutive law is real, symmetric and positive definite (see [36] and section 12.11 of [7]). Also one can introduce a periodic vector potential \mathbf{v} for $\mathbf{j} - \langle \mathbf{j} \rangle$ in (2.13) so that $\mathbf{j} - \langle \mathbf{j} \rangle$ is expressed in terms of the antisymmetric part of $\nabla \mathbf{v}$ using the completely antisymmetric Levi-Civita tensor giving $\mathbf{j} - \langle \mathbf{j} \rangle = \nabla \times \mathbf{v}$, while on the other hand the Levi-Civita tensor applied to ∇V gives an antisymmetric field that has zero divergence. Then the equations can be manipulated into the same form as (2.8)–(2.11) with real $\sigma_j^{(k\ell)} = \sigma_j^{(\ell k)}$.

(a) Equivalence between problems (2.1) and (2.2)

The connection between problems (2.1) and (2.2) is implicit in existing results. To see this, we first consider a problem associated with, and in fact equivalent to, problem (2.2). This is to characterize the G -closure associated with the equations

$$\begin{pmatrix} \mathbf{J}(\mathbf{x}) \\ \mathbf{s}(\mathbf{x}) \end{pmatrix} = \mathbf{K}(\mathbf{x}) \begin{pmatrix} \mathbf{E}(\mathbf{x}) \\ \theta \end{pmatrix}, \quad \mathbf{K}(\mathbf{x}) = [\chi(\mathbf{x})\mathbf{K}_1 + (1 - \chi(\mathbf{x}))\mathbf{K}_2], \quad (2.15)$$

in which $J(x)$ and $E(x)$ satisfy the same constraints as in problem 2.2, K_1 and K_2 are positive definite and given by (2.6), the indicator function $\chi(x)$ is again given by (2.10), but not subject to the constraint that $\langle \chi \rangle = f$, θ is a constant scalar, and $s(x)$ is an arbitrary scalar valued function having the same periodicity as $\chi(x)$. The effective tensor K_* is defined by the linear relation

$$\begin{pmatrix} \langle J \rangle \\ \langle s \rangle \end{pmatrix} = K_* \begin{pmatrix} \langle E \rangle \\ \theta \end{pmatrix}. \quad (2.16)$$

Now when $\theta = 0$ (2.15) when solved for $J(x)$ is exactly the same as (2.8). This implies that K_* takes the form

$$K_* = \begin{pmatrix} L_* & V_* \\ V_*^T & c_* \end{pmatrix}, \quad (2.17)$$

where L_* is the exactly the same effective tensor associated with problem 2.2, defined by (2.12). Furthermore, if we assume that $L_1 - L_2$ is non-singular (by, if necessary, perturbing the problem) then we can find constant fields $J(x) = J_0$ and $E(x) = E_0$ that solve (2.15), and thus obtain formulae for V_* and c_* . This is a standard technique in the theory of composites (see, for example, ch. 5 and in particular section 5.4 in [7] and references therein). Specifically, (2.15) and (2.16) imply

$$\left. \begin{aligned} J_0 &= L_1 E_0 + V_1 \theta = L_2 E_0 + V_2 \theta = L_* E_0 + V_* \theta, \\ \text{and } \langle s \rangle &= [f V_1 + (1-f) V_2]^T E_0 + [f c_1 + (1-f) c_2] \theta = V_* E_0 + c_* \theta, \end{aligned} \right\} \quad (2.18)$$

and these have the solutions

$$\left. \begin{aligned} E_0 &= (L_1 - L_2)^{-1} (V_2 - V_1) \theta, & V_* &= V_1 + (L_1 - L_2)(L_1 - L_2)^{-1} (V_2 - V_1), \\ \text{and } c_* &= f c_1 + (1-f) c_2 + [f V_1 + (1-f) V_2 - V_*]^T (L_1 - L_2)^{-1} (V_2 - V_1). \end{aligned} \right\} \quad (2.19)$$

So c_* and V_* are determined entirely in terms of L_* , f , and the elements of K_1 and K_2 . Conversely, if we know K_* , then from (2.17) we know L_* , V_* and c_* , and the last equation in (2.19) allows us to determine f . Thus solving problem 2.2 is equivalent to solving this problem.

One is often concerned with the quadratic form associated with K_* that sometimes may correspond to the energy stored or dissipated in the material. For constant fields E_0 and θ (with E_0 not restricted to be given by (2.19)) standard variational principles [37] show that

$$\begin{pmatrix} E_0 \\ \theta \end{pmatrix} \cdot K_* \begin{pmatrix} E_0 \\ \theta \end{pmatrix} = \inf_{\mathbf{u}} \left\langle \begin{pmatrix} E_0 + \nabla \mathbf{u} \\ \theta \end{pmatrix} \cdot K(x) \begin{pmatrix} E_0 + \nabla \mathbf{u} \\ \theta \end{pmatrix} \right\rangle. \quad (2.20)$$

If we are interested in the lowest value of this over all $K_* \in G(K_1, K_2)$, normalized with say $\theta = 1$, and use an idea of Kohn [38], we get

$$\begin{aligned} &\inf_{K_* \in G(K_1, K_2)} \begin{pmatrix} E_0 \\ 1 \end{pmatrix} \cdot K_* \begin{pmatrix} E_0 \\ 1 \end{pmatrix} \\ &= \inf_{\chi} \inf_{\mathbf{u}} \left\langle \begin{pmatrix} E_0 + \nabla \mathbf{u} \\ 1 \end{pmatrix} \cdot [\chi(x) K_1 + (1-\chi(x)) K_2] \begin{pmatrix} E_0 + \nabla \mathbf{u} \\ 1 \end{pmatrix} \right\rangle \\ &= \inf_{\mathbf{u}} \left\langle \inf_{\chi} \begin{pmatrix} E_0 + \nabla \mathbf{u} \\ 1 \end{pmatrix} \cdot [\chi(x) K_1 + (1-\chi(x)) K_2] \begin{pmatrix} E_0 + \nabla \mathbf{u} \\ 1 \end{pmatrix} \right\rangle \\ &= \inf_{\mathbf{u}} \left\langle \min_{j=1,2} \begin{pmatrix} E_0 + \nabla \mathbf{u} \\ 1 \end{pmatrix} \cdot K_j \begin{pmatrix} E_0 + \nabla \mathbf{u} \\ 1 \end{pmatrix} \right\rangle \\ &= \inf_{\mathbf{u}} \langle W(E_0 + \nabla \mathbf{u}) \rangle, \end{aligned} \quad (2.21)$$

where $W(\mathbf{F})$ is given by (2.2) and (2.3). So we arrive back at the quasi-convexification of $W(\mathbf{F})$ as in problem 2.1, with $m = n$. If χ is restricted to multiple rank laminate geometries we arrive back

at the rank-one convexification of $W(\mathbf{F})$ (see [39] and section 31.6 of [7]). So problem 2.1 is solved according to whether or not

$$\inf_{\mathbf{K}_* \in G(\mathbf{K}_1, \mathbf{K}_2)} \begin{pmatrix} \mathbf{E}_0 \\ 1 \end{pmatrix} \cdot \mathbf{K}_* \begin{pmatrix} \mathbf{E}_0 \\ 1 \end{pmatrix} = \inf_{\mathbf{K}_* \in G^L(\mathbf{K}_1, \mathbf{K}_2)} \begin{pmatrix} \mathbf{E}_0 \\ 1 \end{pmatrix} \cdot \mathbf{K}_* \begin{pmatrix} \mathbf{E}_0 \\ 1 \end{pmatrix}. \quad (2.22)$$

To have equality it is sufficient, but not necessary, to have $G(\mathbf{K}_1, \mathbf{K}_2) = G^L(\mathbf{K}_1, \mathbf{K}_2)$.

On the other hand, we know the sets $G(\mathbf{L}_1, \mathbf{L}_2)$ and $G^L(\mathbf{L}_1, \mathbf{L}_2)$ have sufficient convexity (as guaranteed by their stability under lamination) to be completely characterized by their ‘W-transforms’. These generalize the idea of the Legendre transform for characterizing convex sets. First note that a linear operator \mathbf{A} on \mathcal{S}_n has elements A_{ijkl} such that if the matrix $\mathbf{C} \in \mathcal{S}_n$ has elements $C_{k\ell}$ then \mathbf{AC} has elements

$$\{\mathbf{AC}\}_{ij} = \sum_{k=1}^2 \sum_{\ell=1}^n A_{ijkl} C_{k\ell}. \quad (2.23)$$

Introducing the inner product

$$\mathbf{A} : \mathbf{B} = \sum_{i,k=1}^2 \sum_{j,\ell=1}^n A_{ijkl} B_{ijkl}, \quad (2.24)$$

between two linear operators \mathbf{A} and \mathbf{B} on \mathcal{S}_n , the W-transform of $G(\mathbf{L}_1, \mathbf{L}_2)$ is

$$W(\mathbf{N}, \mathbf{N}_\perp) = \inf_{\mathbf{L}_* \in G(\mathbf{L}_1, \mathbf{L}_2)} \{\mathbf{N} : \mathbf{L}_* + \mathbf{N}_\perp : \mathbf{L}_*^{-1}\}, \quad (2.25)$$

where \mathbf{N} and \mathbf{N}_\perp range over all real, positive semidefinite, and symmetric operators such that $\mathbf{NN}_\perp = \mathbf{N}_\perp \mathbf{N} = 0$. When $\mathbf{N}_\perp = 0$ and \mathbf{N} is not restricted to be positive semidefinite, this is just the standard Legendre transform. That $G(\mathbf{L}_1, \mathbf{L}_2)$ may be characterized in this way is suggested by results of Cherkaev & Gibiansky [40,41] for particular examples and proved, in general, in [42] (also [43] and section 30.3 of [7], and references therein). Writing

$$\mathbf{N} = \sum_{k=1}^h \mathbf{E}_k \otimes \mathbf{E}_k, \quad \mathbf{N}_\perp = \sum_{k=h+1}^n \mathbf{J}_k \otimes \mathbf{J}_k, \quad (2.26)$$

where some of the \mathbf{E}_k or \mathbf{J}_k could be zero and, without loss of generality, assuming

$$\mathbf{E}_k \cdot \mathbf{E}_\ell = 0, \quad \mathbf{J}_k \cdot \mathbf{J}_\ell = 0, \quad \mathbf{J}_k \cdot \mathbf{E}_\ell = 0, \text{ for all } k \neq \ell, \quad (2.27)$$

we obtain

$$\mathbf{N} : \mathbf{L}_* + \mathbf{N}_\perp : \mathbf{L}_*^{-1} = \sum_{k=1}^h \mathbf{E}_k \cdot \mathbf{L}_* \mathbf{E}_k + \sum_{k=h+1}^n \mathbf{J}_k \cdot \mathbf{L}_*^{-1} \mathbf{J}_k. \quad (2.28)$$

Each of the terms in the first sum can be expressed in variational form, similar to (2.20),

$$\mathbf{E}_k \cdot \mathbf{L}_* \mathbf{E}_k = \inf_{\mathbf{u}_k} \langle [\mathbf{E}_k + \nabla \mathbf{u}_k] \cdot \mathbf{L}(\mathbf{x}) [\mathbf{E}_k + \nabla \mathbf{u}_k] \rangle, \quad (2.29)$$

while the remaining terms in the second sum can be expressed in the dual variational form,

$$\begin{aligned} \mathbf{J}_k \cdot \mathbf{L}_*^{-1} \mathbf{J}_k &= \inf_{\mathbf{v}_k} \langle [\mathbf{J}_k + \mathbf{R}_\perp \nabla \mathbf{v}_k] \cdot [\mathbf{L}(\mathbf{x})]^{-1} [\mathbf{J}_k + \mathbf{R}_\perp \nabla \mathbf{v}_k] \rangle \\ &= \inf_{\mathbf{v}_k} \langle [\mathbf{R}_\perp^T \mathbf{J}_k + \nabla \mathbf{v}_k] \cdot [\mathbf{R}_\perp \mathbf{L}(\mathbf{x}) \mathbf{R}_\perp^T]^{-1} [\mathbf{R}_\perp^T \mathbf{J}_k + \nabla \mathbf{v}_k] \rangle, \end{aligned} \quad (2.30)$$

where the infimum is over all periodic functions \mathbf{v}_k , and

$$\mathbf{R}_\perp = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad (2.31)$$

is the matrix for a 90° rotation. Let us introduce a constant superfield \mathbf{E}_0 and supertensors \mathbf{L}_1 and \mathbf{L}_2 given by

$$\mathbf{E}_0 = \begin{pmatrix} \mathbf{E}_1 \\ \vdots \\ \mathbf{E}_h \\ \mathbf{R}_\perp^T \mathbf{J}_{h+1} \\ \vdots \\ \mathbf{R}_\perp^T \mathbf{J}_n \end{pmatrix}, \quad \mathbf{L}_j = \begin{pmatrix} \mathbf{L}_j & \dots & 0 & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \mathbf{L}_j & 0 & \dots & 0 \\ 0 & \dots & 0 & [\mathbf{R}_\perp \mathbf{L}_j \mathbf{R}_\perp^T]^{-1} & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & 0 & \dots & [\mathbf{R}_\perp \mathbf{L}_j \mathbf{R}_\perp^T]^{-1} \end{pmatrix}. \quad (2.32)$$

Then (2.29) and (2.30) imply

$$(\mathbf{N}, \mathbf{N}_\perp) = \inf_{\underline{\mathbf{u}}} \inf_{j=1,2} \langle \min\{(\mathbf{E}_0 + \nabla \underline{\mathbf{u}}) \cdot \mathbf{L}_j (\mathbf{E}_0 + \nabla \underline{\mathbf{u}})\} \rangle, \quad (2.33)$$

in which the infimum is over all periodic potentials

$$\underline{\mathbf{u}} = \begin{pmatrix} \mathbf{u}_1 \\ \vdots \\ \mathbf{u}_h \\ \mathbf{v}_{h+1} \\ \vdots \\ \mathbf{v}_n \end{pmatrix}. \quad (2.34)$$

Thus finding $G(\mathbf{L}_1, \mathbf{L}_2)$ is reduced to a set of two-well quasi-convexification problems, each indexed by the value of $h = 0, 1, \dots, n$ and with $m = n^2$. The problem of finding $G_f(\mathbf{L}_1, \mathbf{L}_2)$ can be handled in a similar way [42]. Instead of (2.25) one considers

$$W(\mathbf{N}, \mathbf{N}_\perp, c) = \inf_f \inf_{\mathbf{L}_* \in G_f(\mathbf{L}_1, \mathbf{L}_2)} \{ \mathbf{N} : \mathbf{L}_* + \mathbf{N}_\perp : \mathbf{L}_*^{-1} + c \mathbf{I} \}, \quad (2.35)$$

where the constant c acts as a Lagrange multiplier for the volume fraction $f = \langle \chi \rangle$. One easily sees that this again reduces to a two-well quasi-convexification problem.

3. Some open problems related to the effective conductivity as a function of the component conductivities

The lamination closure and the G_f -closure coincide when the block entries of \mathbf{L}_1 and \mathbf{L}_2 are all proportional to the 2×2 identity matrix \mathbf{I} ,

$$\sigma_j^{(k\ell)} = \sigma_j^{(k\ell)} \mathbf{I}, \quad j = 1, 2. \quad (3.1)$$

To see this, we start by following Straley [44] and Milgrom & Shtrikman [45] (see also ch. 6 in [7] and references therein) and introduce a non-singular matrix \mathbf{W} having block entries proportional to \mathbf{I} ,

$$\mathbf{W} = \begin{pmatrix} w^{(11)} \mathbf{I} & w^{(12)} \mathbf{I} & \dots & w^{(1n)} \mathbf{I} \\ w^{(21)} \mathbf{I} & w^{(22)} \mathbf{I} & \dots & w^{(2k)} \mathbf{I} \\ \vdots & \vdots & \ddots & \vdots \\ w^{(n1)} \mathbf{I} & w^{(n2)} \mathbf{I} & \dots & w^{(nn)} \mathbf{I} \end{pmatrix}. \quad (3.2)$$

Now we rewrite (2.8) in the form

$$\underbrace{\mathbf{W}^T \mathbf{J}(\mathbf{x})}_{\mathbf{J}'(\mathbf{x})} = \left[\chi(\mathbf{x}) \underbrace{\mathbf{W}^T \mathbf{L}_1 \mathbf{W}}_{\mathbf{L}'_1} + (1 - \chi(\mathbf{x})) \underbrace{\mathbf{W}^T \mathbf{L}_2 \mathbf{W}}_{\mathbf{L}'_2} \right] \underbrace{\mathbf{W}^{-1} \mathbf{E}(\mathbf{x})}_{\mathbf{E}'(\mathbf{x})}. \quad (3.3)$$

By choosing $\mathbf{W} = \mathbf{L}_2^{-1/2} \mathbf{Q}$ with $\mathbf{Q}^T \mathbf{Q} = \mathbf{I}$ we get $\mathbf{L}_2' = \mathbf{I}$, and then \mathbf{Q} can be chosen so that $\mathbf{L}_1' = \mathbf{Q}^T \mathbf{L}_2^{-1/2} \mathbf{L}_1 \mathbf{L}_2^{-1/2} \mathbf{Q}$ is diagonal, of the form

$$\mathbf{L}_1' = \begin{pmatrix} \sigma^{(1)} \mathbf{I} & 0 & \dots & 0 \\ 0 & \sigma^{(2)} \mathbf{I} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma^{(n)} \mathbf{I} \end{pmatrix}. \quad (3.4)$$

Thus we have reduced the problem down to a set of uncoupled conductivity problems and the associated effective tensor $\mathbf{L}_*^{\prime\prime} = \mathbf{W}^T \mathbf{L}_* \mathbf{W}$ is given by

$$\mathbf{L}_*^{\prime\prime} = \begin{pmatrix} \sigma_*(\sigma^{(1)}) & 0 & \dots & 0 \\ 0 & \sigma_*(\sigma^{(2)}) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_*(\sigma^{(n)}) \end{pmatrix}, \quad (3.5)$$

where $\sigma_*(\sigma)$ is the effective conductivity tensor associated with the equations

$$\mathbf{j}(\mathbf{x}) = [\chi(\mathbf{x})\sigma + (1 - \chi(\mathbf{x}))]\mathbf{e}(\mathbf{x}), \quad \nabla \cdot \mathbf{j} = 0, \quad \mathbf{e} = \mathbf{e}_0 + \nabla V, \quad (3.6)$$

in which $V(\mathbf{x})$ is a periodic potential, and

$$\langle \mathbf{j} \rangle = \sigma_*(\sigma) \langle \mathbf{e} \rangle \quad (3.7)$$

defines the function $\sigma_*(\sigma)$. Allowing for complex values of σ , the properties of this function have been studied in [46–48]. We remark that complex values of σ and hence σ_* or, equivalently, complex values of the dielectric constants of the phases and hence the effective dielectric constant ϵ_* have a physical significance for electromagnetic waves propagating through the structure when the wavelengths and attenuation lengths of the waves in each phase are much larger than the microstructure. This is called the quasi-static regime. In particular, $\text{Im } \epsilon_*$ is related to the energy absorption in the composite, and hence is positive semidefinite when the dielectric constants of the phases are non-negative. Reflecting this, the function $\sigma_*(\sigma)$ satisfies the Nevanlinna–Herglotz type property

$$\text{Im } \sigma_*(\sigma) \geq 0 \quad \text{when } \text{Im } \sigma > 0. \quad (3.8)$$

Additionally, the function is analytic in σ except along the negative real σ -axis, satisfies the constraints that

$$\sigma_*(1) = 1, \quad \left. \frac{d\sigma_*(\sigma)}{d\sigma} \right|_{\sigma=1} = f\mathbf{I}, \quad \sigma_*(\sigma) \geq 0 \quad \text{when } \sigma \text{ is real and positive}, \quad (3.9)$$

and, in two dimensions, the Keller–Dykne–Mendelson relationship [49–51]

$$\sigma_* \left(\frac{1}{\sigma} \right) = \mathbf{R}_\perp [\sigma_*(\sigma)]^{-1} \mathbf{R}_\perp^T, \quad (3.10)$$

where \mathbf{R}_\perp , with transpose \mathbf{R}_\perp^T is the matrix for a 90° rotation given by (2.31). Conversely, any function satisfying these properties can be approximated arbitrarily well by a rational function that corresponds to the effective conductivity function $\sigma_*^L(\sigma)$ of a hierarchical laminate geometry [52] (see also Section 18.5 in [7]). Roughly speaking, given this rational function one can retrieve information about the last two layerings in the corresponding laminate by either setting $\sigma = 0$ or $\sigma = \infty$. One strips this last layering away, and accordingly modifies the associated conductivity function. Then one makes the opposite choice $\sigma = \infty$ or $\sigma = 0$, respectively, and proceeds by induction, until one is left with purely phase 1 or purely phase 2. This establishes that the lamination closure and the G_f -closure coincide when the block entries of \mathbf{L}_1 and \mathbf{L}_2 are all proportional to the 2×2 identity matrix \mathbf{I} . Explicit expressions for the G_f -closure were given in the case $n = 1$ by Lurie & Cherkaev [21] and Murat & Tartar [22] (extended to the three dimensions in [22,53]), in the case $n = 2$ by Cherkaev & Gibiansky [40], and for general n , using the analytic

properties of $\sigma_*(\sigma)$, by Clark & Milton [54]. It is an open question as to whether the G_f -closure for general n can be obtained via the translation method. One can speculate that there should be some sort of inductive procedure using the translation method, but it is difficult to see how to formulate this.

In three dimensions, one would like to address the analogous question, and focusing on isotropic composites this becomes:

Problem 3.1. For three-dimensional isotropic composites, each having an effective conductivity $\sigma_*\mathbf{I}$ and being built from two isotropic materials having conductivities $\sigma\mathbf{I}$ and \mathbf{I} , can one characterize all possible conductivity functions $\sigma_*(\sigma)$?

The conductivity function $\sigma_*(\sigma) = \sigma_*(\sigma)\mathbf{I}$ still satisfies (3.8) and (3.9), but in place of (3.10) it has been established [46,55] that

$$\left. \frac{d^2\sigma_*(\sigma)}{d\sigma^2} \right|_{\sigma=1} = -\frac{2f(1-f)}{3}, \quad (3.11)$$

and, additionally [48,56–59], that the inequality

$$\sigma_*(\sigma)\sigma_*\left(\frac{1}{\sigma}\right) + \frac{\sigma_*(\sigma) + \sigma\sigma_*(1/\sigma)}{\sigma + 1} \geq 2 \quad (3.12)$$

holds for all real positive σ (and is satisfied as an equality for multicoated sphere assemblages). The question is whether there exist additional constraints satisfied by $\sigma_*(\sigma)$, and, if so, to identify them. An associated problem is:

Problem 3.2. For three-dimensional isotropic composites of two isotropic phases, are all possible conductivity functions $\sigma_*(\sigma)$ achievable by multiple rank laminate microstructures and, if so, does it suffice to consider laminate microstructures where one laminates only in mutually orthogonal directions?

We remark that it does not suffice (even in two dimensions) to consider laminate microstructures where one laminates in mutually orthogonal directions if one considers anisotropic composites of two isotropic phases since if σ is complex the real and imaginary parts of $\sigma_*(\sigma)$ do not necessarily commute, while they do commute if one laminates in mutually orthogonal directions.

These results motivate one to consider periodic composites of two anisotropic phases where the conductivity tensor takes the form

$$\sigma(\mathbf{x}) = \chi(\mathbf{x})\sigma_1 + [1 - \chi(\mathbf{x})]\sigma_2, \quad (3.13)$$

where the indicator function $\chi(\mathbf{x})$ is given by (2.10) and σ_1 and σ_2 are the 2×2 matrix-valued conductivity tensors of the two phases. The associated effective conductivity tensor is found by looking for current fields $\mathbf{j}(\mathbf{x})$ and electric fields $\mathbf{e}(\mathbf{x})$, with the same periodicity of the composite, that solve

$$\mathbf{j}(\mathbf{x}) = \sigma(\mathbf{x})\mathbf{e}(\mathbf{x}), \quad \nabla \cdot \mathbf{j} = 0, \quad \mathbf{e} = -\nabla V(\mathbf{x}). \quad (3.14)$$

In these equations, $V(\mathbf{x})$ is the electric potential, and the volume average, $\langle \mathbf{e} \rangle$, of the electric field $\mathbf{e}(\mathbf{x})$ is prescribed. The average current field $\langle \mathbf{j} \rangle$ depends linearly on $\langle \mathbf{e} \rangle$, and it is this linear relation,

$$\langle \mathbf{j} \rangle = \sigma_*(\langle \mathbf{e} \rangle) \quad (3.15)$$

that determines the effective tensor σ_* . We arrive at problem 3.3, again closely related to problems (2.1) and (2.2):

Problem 3.3. For two-dimensional anisotropic composites of two anisotropic phases, are all possible conductivity functions $\sigma_*(\sigma_1, \sigma_2)$ achievable by multiple rank laminate microstructures?

Some progress in characterizing the possible conductivity functions $\sigma_*(\sigma_1, \sigma_2)$ has been made by finding suitable representations of the underlying operators so that they satisfy the required

algebraic properties [60]. Once one has these representations one can, in principle, determine not only $\sigma_*(\sigma_1, \sigma_2)$ but also $L_*(L_1, L_2)$ for all real positive definite L_1 and L_2 taking the block matrix form (2.11). Thus if one could show a direct correspondence between the operator representations for an arbitrary $\chi(x)$ and the operator representations for multiple rank laminate microstructures, one would have resolved problem 2.2, establishing that the G_f -closure equals its lamination closure. Such a correspondence between operator representations was used in [61,62] to establish that in two dimensions the effective conductivity function $\sigma_*(\sigma_0)$ of any polycrystal with conductivity of the form

$$\sigma(x) = R(x)\sigma_0 R^T(x) \quad \text{and} \quad R(x)R^T(x) = I, \quad (3.16)$$

and σ_* given by (3.14) and (3.15), corresponds to the conductivity function of a laminate microstructure.

A question of obvious importance is to identify those two-phase microstructures that absorb as much electromagnetic energy as possible, no matter what the direction of the incident radiation. In the quasi-static limit, where the wavelength of the radiation is much larger than the size of the unit cell of periodicity, the electromagnetic equations decouple into separate electric equations and magnetic equations involving complex fields and complex electrical permittivities and complex magnetic permeabilities, respectively. Each decoupled equation is equivalent to a conductivity equation, with complex conductivities. Four decades ago bounds were derived on the effective complex electrical permittivity (or equivalently the complex magnetic permeability, or complex conductivity) of isotropic composites of two isotropic phases, mixed in fixed proportions [63,64]. The bounds confine the effective electrical permittivity to a lens-shaped region of the complex plane bounded by two circular arcs. The problem becomes one of identifying microstructures that have the maximum imaginary part of the effective complex electrical permittivity. In two dimensions, these are assemblages of doubly coated discs (corresponding to the transverse electrical permittivity of doubly coated cylinders) as they attain the bounds [48]. In three dimensions, new bounds [65] show that assemblages of doubly coated spheres provide one bounding circular arc. The previously known second bounding arc [63,64] corresponds to conductivity functions $\sigma_*(\sigma)$ that have just one pole at a finite negative real value of σ . Originally just five microgeometries were identified that correspond to five points on the circular arc [48]. Depending on the material moduli, these can have the maximum possible absorption. Now an extra three additional multiple rank laminate geometries have been identified with effective electrical permittivities lying on the arc, and which can have the maximum possible absorption [65]. This leads to the following question:

Problem 3.4. Are there other geometries with isotropic effective permittivities that lie on the arc?

There is also a close connection with finding isotropic geometries that attain bounds on the complex effective bulk modulus [66], and which can provide the maximum possible absorption under oscillatory hydrostatic loadings, and that attain bounds coupling the real effective moduli of two conductivity type problems that may separately correspond to say, magnetic, thermal, particle diffusion or fluid permeability problems [46,67]

Another question is the following one:

Problem 3.5. Can any of these discovered geometries, having maximum absorption, be replaced by simpler ones?

In particular, can the assemblages of doubly coated discs or coated spheres be replaced by periodic ones with only one inclusion per unit cell? In the case of assemblages of coated spheres (isotropic composites having the minimum and maximum conductivities for given real positive conductivities of the two phases, mixed in given proportions) equivalent periodic geometries having only one inclusion per unit cell are known [68–70].

4. Bounds on the elastic moduli of an elastic material with voids, and the ultimate auxetic material in this class of materials

Characterizing the possible elasticity tensors of anisotropic composites is a daunting task. Elasticity tensors have 18 invariants in three-dimensional space and five invariants in two dimensions, and correspondingly the set of all possible elasticity tensors built from two isotropic phases in prescribed volume fractions is represented by a set in an 18 or 5, dimensional space, or 21 and 9 if we include the bulk and shear moduli of both phases. The difficulty of this is indicated by the observation that a distorted hypercube in 18 dimensions has $2^{18} \approx 26\,000$ vertices and 18 numbers are needed to specify the coordinates of each, bringing the total to about 4.7 million numbers, just to specify an 18-dimensional distorted cube. The G -closure has only been completely characterized, and consists of all positive definite elasticity tensors, in the limit as one phase becomes arbitrarily compliant while the other phase becomes arbitrarily stiff [23]. A lot of progress has been made in the case where one phase is void, while the other is isotropic with fixed positive elastic moduli, [43] (or when a rigid material replaces the void phase [71]). Still, there are parts of the G -closure that have not been mapped. We arrive at

Problem 4.1. Can one complete the characterization of the G -closure for a void (or rigid) phase mixed with an isotropic elastic phase?

It may be the case that the necessary insight for progressing further, at least in the case that one phase is void, comes from a consideration of the possible pairs of the effective bulk modulus, κ_* , and effective shear modulus μ_* , of isotropic composites of an elastic material, having bulk and shear moduli κ and μ , and void. One has the elementary bounds [37]:

$$0 \leq \kappa_* \leq \kappa, \quad 0 \leq \mu_* \leq \mu. \quad (4.1)$$

Naturally the void has minimum effective bulk and shear moduli, both being zero, and the pure elastic phase has maximum effective bulk and shear moduli. Also one can construct composites with (κ_*, μ_*) arbitrarily close to $(\kappa_*, 0)$ for all positive $\kappa_* < \kappa$, and arbitrarily close to (κ, μ_*) for all positive $\kappa_* < \kappa$ [43,72,73]. On the other hand, the question remains as to what microstructures have high effective shear modulus and low effective bulk modulus. We are led to

Problem 4.2. The bounds (4.1) imply $\mu_* - c\kappa_* \leq \mu$ for all $c > 0$. Can this inequality be improved, in two and/or three dimensions, for a range of $c > 0$? Alternatively, can one construct composites of an elastic phase with void with (κ_*, μ_*) arbitrarily close to $(0, \mu)$?

A related question is

Problem 4.3. Identify, for given $c > 0$, in two and/or three dimensions, isotropic microstructures of an elastic phase with void that have the largest possible value of $\mu_* - c\kappa_*$ (or a sequence of isotropic microstructures with moduli such that $\mu_* - c\kappa_*$ converges to its largest possible value).

When c is extremely large, this amounts to identifying isotropic microstructures that have the largest possible value of μ_* subject to the constraint that κ_* is arbitrarily close to zero. This is what one may call the ultimate auxetic material within the class of materials built from an isotropic elastic phase with voids. Auxetic composites have a negative Poisson's ratio, so that they fatten when they are pulled, corresponding to a ratio $\kappa_*/\mu_* < 2/3$. When one seeks materials built from an isotropic elastic phase with void, that have Poisson's ratios close to the limiting value of -1 and thus with κ_*/μ_* close to zero, it is generally the case that both κ_* and μ_* are very small, not just κ_* . This is a feature of auxetic composites built from rotating elements [74–76] and is less than ideal as one wants to retain shear stiffness.

In two dimensions, one can construct a candidate for the title of the ultimate auxetic material as follows. One first takes the elastic phase and slices it into slabs of uniform thickness with the interfaces perpendicular to the x_1 -axis. The slabs are separated by microstructured layers, very thin compared to the slab thickness. The microstructured layers are such that their only easy

mode of deformation is compression of the layer in the direction x_1 . The thin microstructured layers may, for example, contain the third rank laminate material with a herringbone structure depicted in fig. 13 of [75] or in the second subfigure of fig. 8 in [43]. The macroscopic constitutive relation of the sliced material separated by these microstructured layers, is

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{pmatrix} = \begin{pmatrix} c_{1111} & c_{1122} & 0 \\ c_{1122} & c_{2222} & 0 \\ 0 & 0 & 2c_{1212} \end{pmatrix} \begin{pmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{12} \end{pmatrix}, \quad (4.2)$$

where the σ_{ij} are the Cartesian components of the average stress, while the ϵ_{ij} are the Cartesian components of the average strain. The effective elastic moduli are

$$c_{1111} = \varepsilon, \quad c_{1122} = c\varepsilon, \quad c_{2222} \approx \frac{4\kappa\mu}{\kappa + \mu} = E, \quad c_{1212} \approx \mu, \quad (4.3)$$

where ε is a small parameter, reflecting the easiness of the easy mode of compression in the x_1 -direction, and the appearance of $E = 4\kappa\mu/(\kappa + \mu)$ reflects the fact that the effective Young's modulus for compression in the x_2 -direction is approximately the same as the pure elastic phase, namely E . We now treat this material as a crystal and construct from it the polycrystal with the largest possible effective shear modulus μ_* and smallest possible effective bulk modulus κ_* . According to the bounds and laminate constructions in [77], these are

$$\kappa_* = \frac{c_{1111}c_{2222} - c_{1212}^2}{c_{1111} + c_{2222} - 2c_{1212}}, \quad \text{and} \quad \mu_* = \frac{c_{1111}c_{2222} - c_{1212}^2}{2c_{1212} - 2c_{2222} + 2\sqrt{c_{2222}[c_{1111} + c_{2222} - 2c_{1212} + (c_{1111}c_{2222} - c_{1212}^2)/c_{1212}]}}. \quad (4.4)$$

Substituting (4.3) in these, and taking the limit $\varepsilon \rightarrow 0$ gives

$$\kappa_* = 0, \quad \frac{1}{\mu_*} = \frac{5}{4\mu} + \frac{1}{4\kappa}. \quad (4.5)$$

The formula for μ_* has the required invariance property that if $1/\mu$ and $-1/\kappa$ are shifted by the same constant, then $1/\mu_*$ is shifted by this constant too [78,79]. Owing to this invariance we may assume, without loss of generality, that the initial elastic phase is incompressible ($1/\kappa = 0$) so that (4.5) implies $\mu_* = 4\mu/5$. The question is then:

Problem 4.4. Is $4\mu/5$ the largest possible value of μ_* for a two-dimensional elastic material with voids, given that $\kappa_* = 1/\kappa = 0$?

From a practical standpoint the answer to this question is moot, as not only are such multiple rank laminates impossible to build and subject to buckling, but also the linear elastic moduli are largely irrelevant under finite but small deformations as the microstructured layers will undergo large deformations relative to their thickness. Ideally one wants to address

Problem 4.5. Can one obtain bounds that correlate the possible compressive and shear deformations of composites when these deformations are not infinitesimal?

Returning back to the theoretical problem of finding the ultimate auxetic material, one could use in principle a similar construction in three dimensions. However the barrier is that the polycrystals having the largest μ_* with $\kappa_* = 0$ have not yet been identified. Thus one arrives at

Problem 4.6. What are the possible (κ_*, μ_*) -pairs for three-dimensional isotropic elastic polycrystals (composites built from a single crystal in various orientations)? The bounds of Hill [37] are optimal for κ_* [80], but improved bounds for μ_* or (κ_*, μ_*) pairs are lacking. Hashin & Shtrikman obtained improved bounds on μ_* [81], but only under additional assumptions about crystal orientations, that are not generally valid.

For conductivity the analogous problem has been solved [56,82,83], but the G -closure containing all possible effective conductivity tensors of anisotropic polycrystals has not yet been fully mapped.

More generally, moving back to isotropic composites of two isotropic elastic phases, one possibly rigid or void, the tightest known bounds on the possible (κ_*, μ_*) -pairs are those of Cherkaev & Gibiansky [41], in two dimensions, and those of Berryman & Milton [84], in three dimensions. It seems highly likely that these bounds are not optimal. Gal Shmuel and myself are progressing on a non-trivial route for improving the three-dimensional bounds using the ‘translation method’ approach (see ch. 24 and 25 of [7] and references therein) used by Cherkaev and Gibiansky, but even so these improved bounds are unlikely to be optimal. Thus we come to

Problem 4.7. Can one obtain improved bounds on the elastic moduli pairs of isotropic composites of two isotropic elastic phases, and ultimately find the optimal ones?

Numerical explorations of the possible (κ_*, μ_*) -pairs have been made, for example in [73,85]. From a practical viewpoint, such numerical explorations are probably more useful than the theoretical developments. On the other hand, it is difficult to numerically explore multiscale structures that may be necessary to obtain desired extreme responses, such as in resolving Problem 4.4.

5. Some future directions for wave and other equations

An impressive body of research addresses the problem of bounding the response of bodies to electromagnetic or other waves, and addressing limitations to how one can manipulate these waves. A few examples include the results in [86–90] and references therein. There are many problems to be addressed and new approaches are needed to improve existing bounds, or to reveal novel ones. A framework suited to most linear equations in physics [91–94], including wave and diffusion equations, is to express them in the form

$$\mathbf{J}(\mathbf{x}) = \mathbf{L}(\mathbf{x})\mathbf{E}(\mathbf{x}) - \mathbf{s}(\mathbf{x}), \quad \mathbf{J} \in \mathcal{J}, \quad \mathbf{E} \in \mathcal{E}, \quad (5.1)$$

where the first equation is the constitutive law, with the tensor $\mathbf{L}(\mathbf{x})$ representing the local material properties, $\mathbf{s}(\mathbf{x})$ is the source term, while \mathcal{E} and \mathcal{J} are orthogonal spaces embodying the differential constraints on the fields. Here \mathbf{x} represents a point in space, or space time with x_0 representing time. Scattering problems can also be expressed in this form [95] by incorporating the fields ‘at infinity’ appropriately. The analogue for quadratic forms of quasi-convexity is then Q^* -convexity: a quadratic form $f(\mathbf{P})$ is Q^* -convex if $f(\mathbf{E}) \geq 0$ for all $\mathbf{E} \in \mathcal{E}$. Q^* -convex functions allow one to place bounds on the spectrum of the operator relevant to the problem [96,97]. The subject of Q^* -convexity remains to be explored, and simple examples of Q^* -convex functions need to be found for the various equations, beyond quasi-convex functions and those discovered for the Schrödinger equation (sections 13.6 and 13.7 of [8]). For wave and diffusion equations, it seems likely that they will provide a powerful tool for addressing other bounding problems, and this provides an avenue for future work. In connection with this, variational principles have been developed for acoustic, elastic, and electromagnetic equations at constant frequency in lossy materials [98,99]. These are the direct analogues of those of Cherkaev & Gibiansky [35] that have proved very powerful, in conjunction with the use of quasi-convex functions, for obtaining bounds on the quasi-static response of composites: examples include bounds on effective complex electrical permittivities (section 22.6 of [7,65]) and bounds on complex bulk moduli [66]. So one expects there should be useful bounds resulting from these variational principles for wave equations in lossy media.

Recently it has been discovered that associated with exact relations for composites, as reviewed in ch. 17 of [7] and the book [6], are exact relations satisfied by the infinite body Green’s function in certain inhomogeneous media, and boundary field equalities [100]. Boundary field equalities are exact identities satisfied by the fields at the boundary of the body, given that the fields in the interior of the body satisfy some constraints that do not uniquely determine the interior fields

in terms of their boundary values. A classical example is that a field with zero divergence has zero net flux through the boundary. The theory of these exact relations for Green's function and boundary field equalities extends to wave and diffusion equations [100], or more generally to equations expressible in the form (5.1), but examples, and in particular useful examples, need to be generated.

Another topic to be explored is that of neutral inclusions for wave equations. For static and quasi-static problems, there are many studies of neutral inclusions (see, for example, section 7.11 of [7], the review [101], and references therein). These are inclusions that one can insert in a homogeneous medium without disturbing the surrounding fields, provided these fields fall into an appropriate class. Thus, for example, one may obtain neutrality for a single applied uniform fields, for any uniform field, or for any applied field satisfying the underlying equations. For conductivity, or equivalently for the dielectric problem, coated ellipsoids can be neutral and invisible to any uniform field [102]. In two dimensions, there are other shaped inclusions that can be neutral to a uniform field in a specified direction [103]. Coated dielectric cylinders, where the core, coating, and surrounding medium have dielectric constants of $1, -1 + i\delta$, and 1 become neutral and hence invisible to large classes of fields in the limit $\delta \rightarrow 0$ [104], and can cloak sources and objects [105,106]. Transformations allow one to obtain other inclusions that are neutral and thus invisible to any exterior field, and also cloak objects [107]. The transformation approach also yields neutral inclusions that are invisible to constant frequency electromagnetic waves [108]. Even appropriately coated spheres can be invisible in the far field when the incident is planar [109]. Quite simple inclusions have been found that are neutral and hence invisible to a single incident planar electromagnetic wave [110,111]. One, possibly difficult, research direction, is to explore whether there are other simple geometries, not obtained from a transformation approach, that are invisible to one or more incident plane waves.

Most analysis of wave equations in lossy media has been done at constant frequency, which makes sense as this avoids convolutions in time. However, recent work on bounds in the time domain [112,113] show that it is possible for the temporal response of a two-phase mixture to be untangled at specific times when the applied field has an appropriately tailored dependence on time. This shows it may be productive to depart from focusing on bounds at constant frequency, and to consider bounding responses as a function of time. Beyond the analytic approach used in these papers, the variational approach of Carini & Mattei [114], may be helpful if one can modify it to obtain bounds at each instant in time, rather than to bounding the response over an interval of time.

Data accessibility. This article has no additional data.

Competing interests. I declare I have no competing interests.

Funding. This work was supported by: EPSRC grant no. EP/R014604/1; a Rothschild visiting fellowship at the Newton Institute; and NSF research grant no. DMS-1814854. Additionally, the author is grateful to the National Science Foundation for support through the research grant no. DMS-1814854.

Acknowledgements. The author would like to thank the Isaac Newton Institute for Mathematical Sciences for support and hospitality during the programme 'The Mathematical Design of New Materials' when work on this paper was initiated. Yury Grabovsky is thanked for helpful comments.

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