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Optimization of structural topology in the high-porosity regime

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Abstract

We propose a new approach to topology optimization, based on the use of "single-scale laminates" as structural components. The method is well-founded, because in the high porosity limit these structures achieve maximal stiffness and minimal weight. The method is useful, because the Hooke's law of a single-scale laminate has a simple, explicit formula which scales linearly with weight. And it is interesting, because the selection of relatively simple, manufacturable designs can be addressed using linear or quadratic programming. Our contributions are two-fold: (a) we establish the foundation of this approach, by defining single-scale laminates and giving self-contained proofs of their optimality in the high-porosity limit; and (b) we explore two numerical applications—minimizing weight with a constraint on the Hooke's law, and imposing continuity on a spatially varying microstructure.

Keywords: Extremal microstructures; Effective properties; High-porosity limit; Optimal design; Homogenization

1. Introduction

There is by now a huge literature on the mechanical behavior of porous materials. Attention has often focused on the high-porosity regime—for example trusses, honeycombs, and metal foams. Such structures are of interest as simplified models of naturally occurring composites, and as examples of lightweight materials with desirable material properties. (This introduction is intentionally sparse with references: see Section 2 for links to the relevant literature.)

There is also a huge literature on structural optimization. One theme is the solution of "free material design" problems, in which every Hooke's law is available at an appropriate cost. A second, rather different theme focuses on designs using just two materials, or one material and void. Homogenization-based methods have been used to optimize structural topology, by: (i) identifying optimal microstructures, then (ii) using them to design minimum-weight porous structures subject to compliance constraints.

This paper explores the interface where these topics meet. Our central thesis is that it is fruitful and interesting to focus on structural optimization in the high-porosity regime. This viewpoint is *fruitful* because the optimal microstructures are dramatically simpler in the high-porosity regime. It is *interesting* because the

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optimal microstructures are highly redundant. As a result we must consider rational methods for selecting among equivalent optimal composites; this leads to novel questions of manufacturability and continuous dependence.

A disclaimer is in order: our methods are restricted to problems where stiffness is preferred. Examples of such problems include: (a) minimizing weight subject to an upper bound on the work done by each of several loads; and (b) minimizing weight subject to a lower bound on the first eigenvalue.

We now explain, briefly and informally, why topology optimization is easier in the high-porosity regime than in the general case. The reason is that when stiffness is preferred, it suffices to consider the microstructures we call *single-scale laminates*. A formal definition will be given in Section 3; informally, however, a single-scale laminate consists of finitely many families of beams in $\mathbb{R}^2$ or walls in $\mathbb{R}^3$ (see Fig. 1). We work asymptotically in the limit as the layer thicknesses tend to 0; different families can, however, have different thicknesses. The key properties of single-scale laminates are:

(a) *Superposition Principle*: The Hooke's law of a single-scale laminate is the linear superposition of the (degenerate) Hooke's laws associated with each family of beams or walls.
(b) *Optimality Principle*: Let C be the Hooke's law of a high-porosity composite made from a given elastic material. Then there is a single-scale laminate made from the same material, with the same overall volume fraction of material, whose Hooke's law C_{ssl} satisfies $C_{\mathrm{ssl}} \geqslant C$ in the sense that $\langle C_{\mathrm{ssl}} e, e\rangle \geqslant \langle Ce, e\rangle$ for all e.

(Both statements are asserted only asymptotically, to leading order in the high-porosity limit.) The Optimality Principle permits us to solve optimal design problems by considering only single-scale laminates, and the Superposition Principle makes the resulting optimization tractable. For example, we will show in Section 4.1 how semidefinite programming can be used to minimize weight subject to a constraint on the Hooke's law.

We have always known that optimal designs can be nonunique. For example, in the high-porosity limit a minimum-weight isotropic 2D composite can be achieved using: (i) a triangular lattice; (ii) a Kagomé lattice; (iii) Hashin's concentric circle construction; or (iv) a rank-three sequential laminate. Some authors avoid dealing with this degeneracy by focusing on the Hooke's law rather than the microstructure. Others rely on numerical effects to break the degeneracy. Our focus on single-scale laminates permits a better understanding of the degeneracy, and leads to natural schemes for resolving it. Two such schemes are presented in Section 4:

(a) When the macroscopic Hooke's law is uniform, we use linear programming to maximize the thickness of one family of layers. The resulting single-scale laminates depend continuously on the data and use a minimal number of layers.

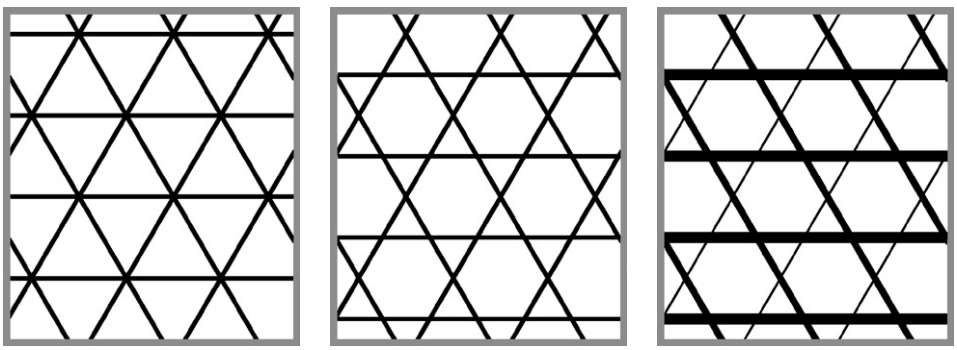

Fig. 1. In 2D, a triangular lattice (left) and a Kagomé lattice (center) are both examples of single-scale laminates; since they have the same layer directions and thicknesses, the Superposition Principle shows they have the same Hooke's law. For a general single-scale laminate, the thicknesses of the layers can depend on their orientation; thus the structure shown on the right is also a 2D single-scale laminate.

(b) When the macroscopic Hooke's law is nonuniform, we use quadratic programming to minimize a suitable norm of the spatial dependence of the single-scale laminates. The resulting layering directions and thicknesses vary smoothly in space.

The term "single-scale laminate" is, we hope, descriptive. But it also serves to highlight the similarities and differences between our work and the established theory of homogenization-based optimal design at fixed volume fraction. There the focus is on microstructures with extremal behavior at fixed volume fraction. For problems in which stiffness is preferred, it is sufficient to consider "sequential laminates." These structures are conceptually simple but physically complex, due to their intrinsically hierarchical structure. Some optimal design problems are known to require such complexity. Our work shows that the high-porosity limit is simpler: in the high-porosity limit, to leading order, hierarchical structure is unnecessary.

Our work has important implications for "free material design." This approach to structural optimization takes the view that any Hooke's law $C \geqslant 0$ is available at an appropriate cost $\Phi(C)$. Therefore semidefinite programming can be used to minimize the total cost $\int \Phi(C(x))\,dx$ subject to constraints on the mechanical response of the associated structure. But how should one choose the cost Φ? For algorithm development and proof of concept, it was natural to use something simple, like an isotropic norm of C. Our work shows that if the goal is topology optimization in the high-porosity regime, then $\Phi(C)$ should be the minimum weight of a single-scale laminate that's greater or equal to C—which, though not explicit, is readily available numerically (Section 4.1).

Our work has antecedents of course. Versions of the Superposition Principle have been noted by various authors, e.g. Cioranescu and Saint Jean Paulin (1999) and Christensen (1986). In 2D, compliance optimization under a single load leads in the high-porosity limit to Michell trusses, a special class of single-scale laminates (Allaire and Kohn, 1993b; Bendsøe and Haber, 1993). In 3D, it has long been recognized that optimality requires a closed-cell structure made from walls, not an open-cell structure made from trusses.

The plan of this paper is as follows. Section 2 surveys relevant literature, elaborating on the connections noted above. Section 3 defines the class of single-scale laminates more precisely, and gives more careful statements of the Superposition and Optimality Principles. Section 4 presents our numerical applications: finding minimum-weight single-scale laminates by semidefinite programming (Section 4.1), then finding simpler minimum-weight structures by two alternative selection mechanisms (Sections 4.2 and 4.3). Finally, Section 5 provides proofs of the Superposition (Section 5.1) and Optimality (Section 5.2) Principles, and draws a connection between single-scale and sequential laminates (Section 5.3).

2. Context

There is a huge literature on the mechanical modelling of high-porosity structures. There is also a huge literature on structural optimization. This section is not intended to survey either field, but rather to put our results in context.

2.1. The mechanics of high-porosity structures

A porous structure is, for our purposes, a high-porosity mixture of a nondegenerate elastic material and void. The analysis of such structures is considered at length in the monographs by Gibson and Ashby (1997) and Cioranescu and Saint Jean Paulin (1999); see also Christensen (2000) for a recent review. A version of our Superposition Principle is proved for 2D structures in Cioranescu and Saint Jean Paulin (1999) (Chapter 2, Section 1.3) by direct examination of the "cell problem." The principle itself seems, however, to be much older. For example, it is used by Christensen (1986) to estimate the Hooke's law of an isotropic closed-cell or open-cell foam (and he refers there to similar calculations as early as 1952).

Highly regular structures such as lattices and honeycombs have naturally received special attention. In two space dimensions, it is well-known that a triangular lattice achieves the Hashin–Shtrikman upper bound on both bulk and shear moduli, to leading order in volume fraction. Hyun and Torquato (2002) noted that this is also true for a Kagomé lattice, and they looked numerically at the relation between stiffness and weight for such structures as the porosity decreases.

The work just cited uses periodic homogenization, keeping the structure of the unit cell fixed as the length scale tends to zero. Our work uses the same viewpoint. When the structure of the unit cell is permitted to change, Zhikov (2002) has shown that new phenomena can occur; for example, the limit problem can be nonlocal. It would be interesting to investigate whether the larger family of limits achievable this way might do better than the "optimal" designs considered here. We think not, because for compliance optimization a relaxation-based viewpoint gives the same result as one based on standard homogenization (Allaire and Francfort, 1998).

2.2. Homogenization-based optimal design

Homogenization-based optimal design dates from the 1970s. Our viewpoint is most like that of Allaire (2002); additional background and context can be found in Bendsøe (1995), Cherkaev and Kohn (1997), and Cherkaev (2000). The basic idea is to break the task of optimal design into two parts:

(a) *characterize the possible composites* by identifying, for each $0<\theta<1$, the set G_θ of Hooke's laws achievable with volume fraction θ; then
(b) *employ optimal sizing methods* to determine the optimal use of these materials for the mechanical problem at hand.

The mathematical theory mainly applies to mixtures of nondegenerate materials; to consider porous structures, we can consider mixtures of two materials then take the limit in which the Hooke's law of the more compliant material tends to zero.

For problems where stiffness is preferred—for example minimizing weight subject to upper bounds on the work done by finitely many specified loads—it is not necessary to characterize *all* possible composites. Rather, it suffices to characterize the "stiffest" elements of G_θ. A key result, due to Avellaneda (1987), is that it suffices for this purpose to consider "sequential laminates." (This class of microstructures had been considered earlier in special cases, but the first systematic and general discussion for elasticity was given by Francfort and Murat (1986).)

Sequential laminates are hierarchical structures, whose description (and, if possible, manufacture) requires consideration of two or more well-separated microstructural length scales. In some cases the same (extremal) properties can be achieved using single-scale microstructures such as the "Vigdergauz construction" (Grabovsky and Kohn, 1995; Vigdergauz, 1994). In other cases, however, this is false: Allaire and Aubry (1999) have shown that some extremal Hooke's laws are achievable *only* by sequential laminates. A central point of the present article is that the situation is different, for porous composites in the high-porosity limit. Our single-scale laminates are, more or less, sequential laminates without the separation of scale. Our Superposition Principle reveals that the separation of scales is irrelevant to leading order as the volume fraction of material approaches zero.

We note in passing that there are interesting optimal design problems for which stiffness is *not* preferred, for example the design of compliant mechanisms (Sigmund, 1997). Such problems require methods other than those of the present paper.

2.3. Free material design

When the goal is to minimize weight subject to compliance constraints, the two-step procedure of homogenization-based optimal design can be organized a bit differently:

(a) first identify, for any achievable Hooke's law, the minimum volume fraction required to achieve it; then
(b) minimize weight among all structures meeting the compliance constraints.

Part (a) is difficult, and some authors have suggested it is also unnecessary. The approach known as "free material design" permits designs using *any* positive semidefinite tensor as a Hooke's law, and specifies the cost of Hooke's law C (usually an isotropic norm of C) as part of the model. Originally introduced by Bendsøe

et al. (1994), it has attracted much attention as an application of semidefinite programming, see e.g. Ben-Tal et al. (1999). Our work shows how the cost function can be chosen to make "free material design" equivalent to the high-porosity limit of homogenization-based optimal design (see Section 4.1).

2.4. Optimal design in the low-volume-fraction limit

We are naturally not the first to study optimal design in the high-porosity regime. One approach is to consider trusses with many possible nodes and members, optimizing numerically, see e.g. Ben-Tal and Nemirovski (1997). A second approach is to examine the homogenization-based approach in the high-porosity limit, see Allaire and Kohn (1993b) and Bendsøe and Haber (1993). Remarkably, for compliance optimization under a single load in two space dimensions, both these approaches reduce to the study of Michell trusses (Michell, 1904). In three space dimensions, however, the high-porosity limit of homogenization is *different* from the study of Michell trusses. In fact an optimal structure should be made from walls not struts. This is clear from looking at the optimal microstructures, cf. Allaire and Kohn (1993b). In addition it is quite intuitive: a wall does better than two orthogonal families of struts lying in the same plane, because each point of the wall does double duty—transmitting stress in both directions.

The viewpoint of the present article amounts to: (i) considering composites made from two nondegenerate materials, then (ii) letting one material become degenerate, then finally (iii) letting the volume fraction of the remaining material tend to zero. We already noted in Section 2.1 that some limits of porous structures cannot be obtained this way. Recent work by Bouchitté, Buttazzo, and Fragalà aims to develop a more general analytical framework for structural optimization of low-dimensional structures, see Bouchitté (2003), Bouchitté and Buttazzo (2001), and Bouchitté et al. (2002).

3. Definition and properties of single-scale laminates

According to the Superposition Principle, the Hooke's law of a single-scale laminate is the linear superposition of the Hooke's laws associated with each family of layers. It is therefore natural to begin, in Section 3.1, by discussing the Hooke's law of a single family of layers. We then proceed, in Section 3.2, to give precise statements of the Superposition and Optimality Principles.

3.1. The linear algebra of layering

Layered composites have been studied by many authors. The goal of this subsection is to give a concise formula for the (degenerate) Hooke's law C of the layered composite obtained by mixing volume fraction θ of Hooke's law A with volume fraction $1-\theta$ of void, in layers orthogonal to a fixed vector k.

If A is isotropic this is a very standard calculation. In terms of the Lamé moduli λ and μ, (i.e. if $A\xi = 2\mu\xi + \lambda(\operatorname{tr}\xi)I$), the composite's Hooke's law C satisfies

$$\langle C\xi,\xi\rangle = \theta\left(\langle A\xi,\xi\rangle - \frac{1}{\mu}\frac{|A\xi k|^2}{|k|^2} + \frac{\lambda+\mu}{\mu(\lambda+2\mu)}\frac{\langle A\xi k,k\rangle^2}{|k|^4}\right). \tag{1}$$

This is a special case of formula (5) below.

Remarkably, when A is anisotropic a simple formula is still possible. This may at first seem an academic exercise, since for applications to optimal design it is natural to take A isotropic. But actually the extension is quite useful: permitting A to be an arbitrary Hooke's law simplifies the notation. We shall use the notation of Allaire (2002), adopting the projection-based viewpoint of Allaire and Kohn (1993a). (Allaire's book emphasizes the case when A is isotropic, but one sees from the 1993 Allaire–Kohn paper that the case of anisotropic A is no different.) The following calculation is, however, older than these references: it was first done for conductivity in Tartar (1985) and for elasticity in Francfort and Murat (1986).

We begin with some notation: if $\mathscr{M}_N$ is the space of all $N\times N$ symmetric matrices and k is any nonzero vector, let $W(k)$ be the subspace

$$W(k) = \{\eta\in\mathscr{M}_N;\eta\cdot k = 0\}. \tag{2}$$

(We think of this as the space of stresses compatible with layering direction k; here $\eta \cdot k$ is the product of the matrix η times the vector k.) The orthogonal complement of $W(k)$ is

$$V(k) = \{\xi \in \mathscr{M}_N; \exists a \in \mathbb{R}^N \text{ such that } \xi = a \odot k\}, \tag{3}$$

where $a \odot k = \frac{1}{2}(a \otimes k + k \otimes a)$.

For any (nondegenerate) Hooke's law A, we have the orthogonal decomposition

$$\mathscr{M}_N = A^{1/2}V(k) \oplus A^{-1/2}W(k). \tag{4}$$

In other words, any ξ can be expressed uniquely as $\xi = A^{1/2}v + A^{-1/2}w$ with $v \in V(k)$ and $w \in W(k)$. We write $\Pi_{A^{1/2}V(k)}\xi$ and $\Pi_{A^{-1/2}W(k)}\xi$ for the orthogonal projections of ξ on these two subspaces.

We are ready to state the extension of Eq. (1) to anisotropic A: the Hooke's law of the layered composite mixing A with void in layers normal to k is $C = \theta f_A^c(k)$ where θ is the volume fraction of A and

$$f_A^c(k) = A^{1/2}\Pi_{A^{-1/2}W(k)}A^{1/2}. \tag{5}$$

In other words, the elastic energy quadratic form of the composite is

$$\langle C\xi, \xi\rangle = \theta\langle A^{1/2}\Pi_{A^{-1/2}W(k)}A^{1/2}\xi, \xi\rangle.$$

When A is isotropic, this reduces to Eq. (1). (An easy way to see this is to set $A\eta = 2\mu\eta + \lambda(\operatorname{tr}\eta)I$ in Eq. (7) below, then do the indicated minimization over $v \in V(k)$.)

To explain the origin of Eq. (5), we start from fact that for the composite made by layering two materials A and B in layers perpendicular to k with volume fractions θ and $1-\theta$, the effective energy quadratic form is

$$\min_{\substack{\xi=\theta\xi_A+(1-\theta)\xi_B \\ \xi_B-\xi_A\in V(k)}} \theta\langle A\xi_A, \xi_A\rangle + (1-\theta)\langle B\xi_B, \xi_B\rangle. \tag{6}$$

The first constraint is equivalent to

$$\xi_A = \xi - (1-\theta)(\xi_B - \xi_A), \quad \xi_B = \xi + \theta(\xi_B - \xi_A)$$

and from the second constraint $(1-\theta)(\xi_B - \xi_A)$ can be any element of $V(k)$. Therefore, Eq. (6) is equivalent to

$$\min_{v\in V(k)} \theta\langle A(\xi+v), \xi+v\rangle + (1-\theta)\left\langle B\left(\xi - \frac{\theta}{1-\theta}v\right), \xi - \frac{\theta}{1-\theta}v\right\rangle.$$

When $B = 0$ we are left with

$$\min_{v\in V(k)} \theta\langle A(\xi+v), \xi+v\rangle. \tag{7}$$

The optimal v is such that $A(\xi+v) \perp V(k)$, or equivalently $A^{1/2}(\xi+v) \perp A^{1/2}V(k)$. Comparing this with the relation $A^{1/2}\xi = \Pi_{A^{1/2}V(k)}A^{1/2}\xi + \Pi_{A^{-1/2}W(k)}A^{1/2}\xi$ we see that when v is optimal for (7),

$$A^{1/2}v = -\Pi_{A^{1/2}V(k)}A^{1/2}\xi \quad \text{and} \quad A^{1/2}(\xi+v) = \Pi_{A^{-1/2}W(k)}A^{1/2}\xi.$$

Therefore

$$\langle A(\xi+v), \xi+v\rangle = \|\Pi_{A^{-1/2}W(k)}A^{1/2}\xi\|^2 = \langle A^{1/2}\Pi_{A^{-1/2}W(k)}A^{1/2}\xi, \xi\rangle.$$

Thus Eq. (7) is equal to $\theta\langle f_A^c(k)\xi, \xi\rangle$, with $f_A^c(k)$ defined by (5).

We note for later use (in Section 5) that $V(k)$, $W(k)$, and $f_A^c(k)$ depend only on $k/|k|$, and that

$$f_A^c(k) = A - Af_A(k)A, \tag{8}$$

where

$$f_A(k)\xi = A^{-1/2}\Pi_{A^{1/2}V(k)}A^{-1/2}\xi. \tag{9}$$

3.2. Single-scale laminates

A single-scale laminate is a high-porosity structure made from a fixed material A. It consists of finitely many families of parallel beams in $\mathbb{R}^2$, or finitely many families of parallel walls in $\mathbb{R}^3$. The structure is determined by

(a) its *rank*: the number of families, an integer $p \geqslant 1$;
(b) its *layer normals*: unit vectors $k_1, \ldots, k_p$, assumed distinct (i.e. $k_i \neq \pm k_j$ for $i \neq j$);
(c) its *layer proportions*: positive real numbers $t_1, \ldots, t_p$ with $\sum_{i=1}^{p} t_i = 1$.

We are interested in the high-porosity limit, so there is also a *scale factor* θ, representing (to leading order) the volume fraction of material. The physical structure of interest consists of *layers of thickness* θt_i *normal to* k_i, $1 \leqslant i \leqslant p$.

The actual geometry of the composite is not fully determined by these parameters. For example, a triangular lattice and a Kagomé lattice have the same layer normals and proportions (see Fig. 1). We shall prove, however, that to leading order as $\theta \to 0$, the Hooke's law of such a composite depends only on the layering normals and proportions. Therefore, it is not useful to distinguish between different structures with the same layer normals and proportions.

The base material A can be isotropic or anisotropic. In the anisotropic case, however, we assume its orientation is fixed. (Thus the orientation is not permitted to depend on the layer normal.)

Our focus is on the linearly elastic behavior of this porous composite. If the layering directions are rationally related then the structure is spatially periodic, with a (possibly large) period cell. The general case can be approximated by such structures, so periodic homogenization is sufficient for proving theorems about the effective behavior. In this setting the local Hooke's law is A where there is material and 0 where there is not; in other words it equals $\chi(y)A$ where χ is a periodic function taking only values 0 and 1. Evidently

$$\chi = \sum_{i=1}^{p} \chi_i - g^{(\mathrm{ov})}, \tag{10}$$

where χ_i is the characteristic function of the ith family of layers (a periodic function of $y \cdot k_i$, taking only the values 0 and 1, with average value θt_i) and $g^{(\mathrm{ov})}$ is supported in the region where the layers overlap. The overlap term is bounded by the number of families ($0 \leqslant g^{(\mathrm{ov})} \leqslant p$) and the volume of its support is of order θ^2, so

$$\int_Y |g^{(\mathrm{ov})}(x)| \, \mathrm{d}x = \mathcal{O}(\theta^2).$$

Our focus is on the leading-order behavior as $\theta \to 0$; therefore quantities of order θ^2 will always be treated as error terms.

Having defined the notion of a single-scale laminate, we now give careful statements of the Superposition and Optimality Principles:

(1) *Superposition Principle*: Let $C_p^{(\mathrm{s})}$ be the effective Hooke's law of a rank-p single-scale laminate with normals $\{k_i\}_{i=1}^p$, proportions $\{t_i\}_{i=1}^p$, and scale factor θ. Then

$$C_p^{(\mathrm{s})} = \theta \sum_{i=1}^{p} t_i f_A^{\mathrm{c}}(k_i) + \mathcal{O}(\theta^2). \tag{11}$$

(2) *Optimality Principle*: Let C be the effective Hooke's law of a high-porosity composite made by mixing a fixed material A with void, in volume fractions θ and $1-\theta$, respectively. Then there exists a single-scale laminate $C_+^{(\mathrm{s})}$ with same volume fraction that is at least as stiff in the sense that

$$C \leqslant C_+^{(\mathrm{s})} + \mathcal{O}(\theta^2). \tag{12}$$

The proofs will be given in Section 5, but let us make a few comments here. Concerning the Superposition Principle: if the different families of layers did not intersect then superposition would be obvious. But they do intersect, and this appears to impose a kinematic constraint linking the elastic deformations of the distinct families of layers. In proving the Superposition Principle, we will effectively be showing that this constraint is not important in the high porosity limit. Concerning the Optimality Principle: an analogous statement is known for sequential laminates. Therefore, the principle can be proved by either: (a) comparing the Hooke's law of a single-scale laminate with that of the associated sequential laminate—showing that the two agree to leading order in θ; or (b) repeating the arguments used for sequential laminates in the context of single-scale laminates. The latter approach turns out to be easier, but we also discuss the former since the connection between sequential and single-scale laminates is of independent interest.

It is natural to wonder whether the layers might buckle. The analysis of buckling in elastic composites is complicated, because buckling can be initiated at any length scale (microscopic, macroscopic, or in between). We do not attempt to address it here, except to note that buckling seems unlikely if the stresses in the layers are tensile. Our analysis in Section 5 gives more than just the Hooke's law of the composite—it also identifies the stress in each layer. Thus it gives sufficient information to check a criterion for microbuckling.

Our attention is on the high-porosity limit, so we often ignore terms of order θ^2 and drop the scale factor θ. Thus, in Section 4 where we focus on the optimal selection of single-scale laminates, we take the view that the Hooke's law of a single-scale laminate is

$$\sum_{i=1}^{p} t_i f_A^{\mathrm{c}}(k_i). \tag{13}$$

Note that the set of possible Hooke's laws (13) is precisely the convex hull of $\{f_A^{\mathrm{c}}(k)\}$ as k ranges over the unit sphere.

Because Eq. (13) is linear, there are in general many single-scale laminates with a given Hooke's law. For example, if A is isotropic and we work in 2D, any rotation of a triangular lattice gives the same isotropic Hooke's law. Moreover, if two single-scale laminates give the same Hooke's law

$$\sum_{i=1}^{p} t_i f_A^{\mathrm{c}}(k_i) = \sum_{j=1}^{q} s_j f_A^{\mathrm{c}}(n_j)$$

then so does any affine combination (using proportions αt_i for layer normals $\{k_i\}$ and proportions $(1-\alpha)s_j$ for layer normals $\{n_j\}$, $0<\alpha<1$). By a suitable limiting procedure, one can also consider structures with a continuum of layering directions. Returning to our previous example, if A is isotropic in 2D, then besides rotated triangular lattices, we also get an isotropic Hooke's law by taking the layer directions to be uniformly distributed on the unit circle.

4. Numerical applications

Many pages have been devoted to bounds on the effective moduli of composites. These bounds determine, at least implicitly, the minimum density a porous composite must have to achieve a specified stiffness. But extracting this information numerically is not an easy matter. Moreover, though the theory supplies microstructures achieving the bounds, they are typically sequential laminates, which are difficult or impossible to manufacture due to the requirement of multiple length scales. When the theory offers us simpler structures (e.g. Hashin's concentric sphere construction, or the Vigdergauz microstructure) there is no systematic method for classifying or choosing between them. Numerical structural optimization has been used to find extremal microstructures, for example by Sigmund (1994), but again the task is difficult and its solution is unsystematic.

Optimal design in the high-porosity regime is, by contrast, dramatically simpler. This is because the only composites we need to consider are single-scale laminates (for applications where stiffness is preferred).

This section demonstrates the extent of the simplification by discussing three simple but practical problems:

(a) finding the minimum density required for a given stiffness, as an application of semidefinite programming (Section 4.1);

(b) finding the "simplest" single-scale laminate with a given Hooke's law, as an application of linear programming (Section 4.2); and
(c) finding a continuously varying family of single-scale laminates that achieve a continuously varying family of Hooke's laws, as an application of quadratic programming (Section 4.3).

We elaborate briefly on (b) and (c). It is no surprise that many different structures have the same Hooke's law. This is clear from counting parameters (the class of all structures has many more degrees of freedom than the class of all Hooke's laws). The resulting redundancy is a gift from nature: it permits us to optimize the elastic response (which involves only the Hooke's law) and also *something else*. There are many reasonable choices for the secondary criterion. We focus in (b) and (c) on "simplicity" and "continuity," since these properties are clearly desirable for manufacturability.

4.1. Minimizing density

We address the following problem: given a Hooke's law C_0, find a microstructure S and its associated Hooke's law C_S solving

$$\min\{\text{density}(S);\ C_S \geqslant C_0,\ C_S \text{ achieved by the microstructure } S\}. \tag{14}$$

In the high-porosity regime, it suffices by the Optimality Principle to consider microstructures in the class of single-scale laminates. Therefore, Eq. (14) reduces to the optimization

$$\min_{\substack{\tau_1,\dots,\tau_p \geqslant 0 \\ k_1,\dots,k_p \in \mathbb{S}^{N-1} \\ \sum_{i=1}^p \tau_i f_A^{\mathrm{c}}(k_i) \geqslant C_0}} \sum_{i=1}^p \tau_i. \tag{15}$$

Here, $N = 2$ for 2D structures and $N = 3$ for 3D structures ($\mathbb{S}^{N-1}$ is the unit circle in $\mathbb{R}^2$ when $N = 2$ and the unit sphere in $\mathbb{R}^3$ when $N = 3$). The constraint $\sum_{i=1}^p \tau_i f_A^{\mathrm{c}}(k_i) \geqslant C_0$ means that the associated quadratic forms are well-ordered:

$$\left\langle \sum_{i=1}^p \tau_i f_A^{\mathrm{c}}(k_i)\xi, \xi \right\rangle \geqslant \langle C_0\xi, \xi\rangle \tag{16}$$

for any $N \times N$ symmetric matrix ξ. The parameters $\{\tau_i\}$ represent $\{\theta t_i\}$; thus the single-scale laminate has density $\theta = \sum \tau_i$ and layering proportions $t_i = \tau_i/\theta$.

The rank of the single-scale laminate (the value of p) seems at first to be part of the optimization. However, it is easy to see that p need not be large, since each point in the convex hull of $\{f_A^{\mathrm{c}}(k)\}_{k\in\mathbb{S}^{N-1}}$ is a convex combination of at most $d+1$ extreme points, where $d = d(N)$ is the dimension of the space of Hooke's laws. (If A is isotropic—the case of primary physical interest—one can do better: using the special form of $f_A^{\mathrm{c}}(k)$ in that case, Francfort et al. (1995) have shown that it suffices to consider $p = 3$ in two space dimensions and $p = 6$ in 3D.)

We want to solve Eq. (15) numerically. One could imagine taking the theoretical minimum value of p and optimizing over the $\tau_1,\dots,\tau_p$ and $k_1,\dots,k_p$. This is not very convenient, however, since the stiffness constraint is nonlinear in k_i.

Our approach is different. Since k_i can be any unit vector and p can be large, we view the expression $\sum_{i=1}^p \tau_i f_A^{\mathrm{c}}(k_i)$ as a discretized integral over the unit sphere of a function $\tau(k) f_A^{\mathrm{c}}(k)$. Discretizing systematically, we let k range over a large but fixed set of M unit vectors $k_1,\dots,k_M$ (equispaced on the unit circle in $\mathbb{R}^2$, or approximately equispaced on the unit sphere in $\mathbb{R}^3$). Our numerical problem is thus

$$\min_{\substack{\tau_1,\dots,\tau_M \geqslant 0 \\ \sum_{i=1}^M \tau_i f_A^{\mathrm{c}}(k_i) \geqslant C_0}} \sum_{i=1}^M \tau_i. \tag{17}$$

Since the layering directions have been fixed, the optimization is only over $\tau_1,\dots,\tau_M$.

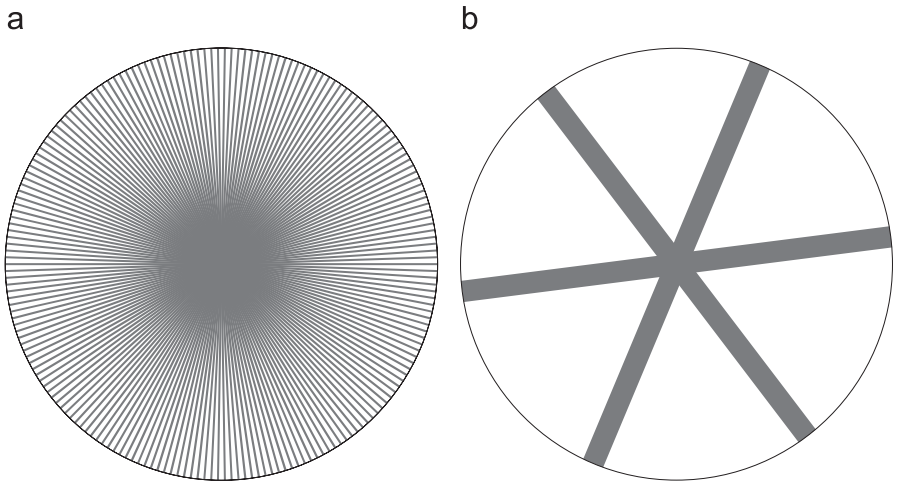

Fig. 2. Minimum-density single-scale laminates in two space dimensions, i.e. solutions of Eq. (14). The Hooke's law C_0 was chosen to be isotropic with Lamé moduli $\lambda = 1$ and $\mu = 0.5$. The underlying elastic material was also chosen isotropic, also with Lamé moduli $\lambda = 1$ and $\mu = 0.5$. The half-unit-circle was discretized by $M = 100$ equispaced directions. Each figure shows the layer thicknesses of the associated single-scale laminate by superimposing segments of thickness τ_i and normal k_i: (a) Result of the semidefinite program discussed in Section 4.1; (b) simplification via linear programming, as discussed in Section 4.2.

The positivity constraint (16) is linear with respect to τ_i, so Eq. (17) has the form of a *semi-definite program* (see for example Vandenberghe and Boyd, 1996). Efficient algorithms and software have been developed for such problems in recent years using interior-point methods. The semidefinite programs solved in this paper were all done using the SP software package, originally developed by Vandenberghe and Boyd.

Fig. 2(a) shows the solution of Eq. (17) obtained by semidefinite programming in two space dimensions with C_0 is isotropic. The half-unit circle was discretized by $M = 100$ equispaced orientations. Each line in the figure has normal k_i and thickness τ_i.

We observed in Section 3.2 that there are many different single-scale laminates with the same isotropic Hooke's law and the same (minimal) weight. As the figure shows, our semidefinite programming approach selects the one that uses all the available layering directions with equal weights. This is not surprising, given the symmetry of the problem and the interior-point character of the algorithm. Additional examples of semidefinite programming (with C_0 orthotropic) will be discussed in Section 4.3 (see Figs. 3(a)–(c)). Those examples confirm that our approach via semidefinite programming usually produces relatively uniform structures, using many if not all the available layering directions.

4.2. Maximizing simplicity

Since many single-scale laminates have the same Hooke's law, it is natural to select a particular solution by optimizing something else. If the goal is manufacturability, it seems natural to look for a structure with relatively few layering directions.

This goal can be achieved by conventional linear programming. Continuing our focus on minimal density, suppose C_1 is the Hooke's law of an optimal single-scale laminate (obtained by semidefinite programming as explained above) and $\theta = \sum_{i=1}^{M} \tau_i$ is its density. We seek another single-scale laminate with the same Hooke's law and density but just a few active layers. To find it, we *maximize the thickness in a particular direction*. Specifically, if the initially given single-scale laminate has maximal thickness in layering direction k_l, we solve

$$\max_{\substack{\tau_1,\ldots,\tau_M \geqslant 0 \\ \sum_{i=1}^{M} \tau_i = \theta \\ \sum_{i=1}^{M} \tau_i f_A^{c}(k_i) = C_1}} \tau_l. \tag{18}$$

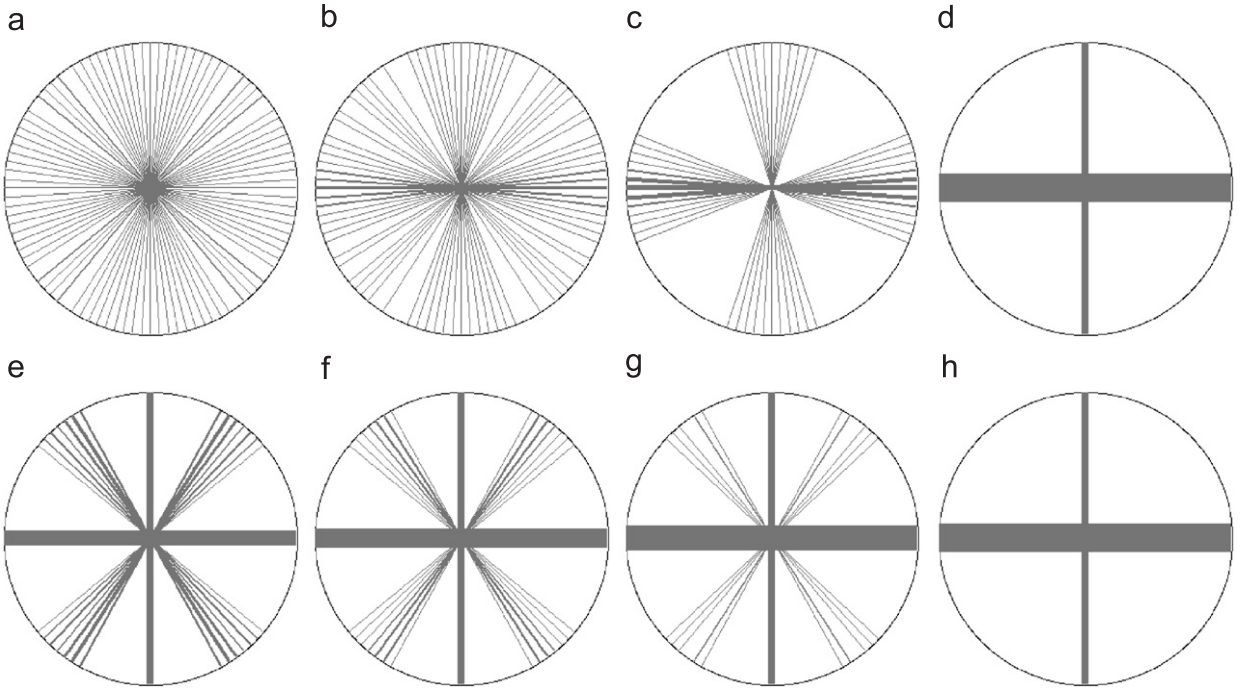

Fig. 3. Selection of single-scale laminates, when the Hooke's law varies linearly between an isotropic law and an orthotropic one. Top row: outcome of the semidefinite program from Section 4.1. Bottom row: outcome of the quadratic program (19).

Since the stiffness constraint is now linear, this is a *linear program*. It can be solved by the simplex method. Since simplex method always returns a vertex of the feasible set, the solution will have most of its layering parameters τ_i equal to zero—indeed (barring degeneracy) it will *minimize* the number of active directions. This is what is observed numerically. For example, when C_1 is isotropic the resulting single-scale composite uses just three equispaced layering directions, corresponding to a triangular or Kagomé lattice (see Fig. 2(b)).

4.3. Enforcing continuity

The preceding examples address the optimal design of macroscopically uniform microstructures. We turn now to a different type of problem: the optimal design of a macroscopically heterogeneous structure.

The starting point we have in mind is the output of a homogenization-based or free-material-design-based design algorithm. It would specify the desired Hooke's law and density as a function of position in the design domain. To pass from this information to an actual design, one must "fill in the microstructure" by specifying, for each point in the design domain, a microstructure with the proposed Hooke's law and density. These structures can then be pieced together. Thinking numerically: if the macroscopic Hooke's law is piecewise constant on a triangulation of the design domain, then each triangle would be filled with a uniform microstructure achieving the desired properties.

If the macroscopic structure varies smoothly, it is natural to ask that the microstructure also vary smoothly. We shall explain how this can be achieved within the class of single-scale laminates by solving a quadratic program.

To capture the main idea in the simplest possible setting, we suppose the macroscopic Hooke's law C and density θ depend only on one coordinate x_1, taking values $\{C_j\}_{j=1}^K$ and $\{\theta_j\}_{j=1}^K$ at evenly spaced nodes along the x_1 axis. We also suppose these Hooke's laws and densities are achievable by single-scale laminates. (If not, we would solve Eq. (14)—or more precisely Eq. (17)—at each node, to replace C_j with a Hooke's law that is at least as stiff, at least as light, and achievable by a single-scale laminate.)

Our strategy is simple. We work, as in Sections 4.1 and 4.2, with single-scale laminates using a fixed collection of layer normals $\{k_i\}_{i=1}^M$. The single-scale laminate at node j is described by its vector of layer thicknesses $\tau^j = (\tau_1^j, \ldots, \tau_M^j)$. To achieve continuous dependence, we will minimize the "Dirichlet norm" of the spatial variation

$$\sum_{j=1}^{K} \left\{ \sum_{i \text{ neighbor of } j} d^2(\tau^i, \tau^j) \right\} \tag{19}$$

where $d(\tau, \tau')$ measures the "distance" between the single-scale laminates associated with τ and τ'. The optimization is over the layering parameters at all nodes, $\tau_k^j \geqslant 0$, $1 \leqslant j \leqslant K$, $1 \leqslant k \leqslant M$, subject to constraints on the density and Hooke's law at each node:

$$\sum_{i=1}^{M} \tau_i^j = \theta_j, \quad 1 \leqslant j \leqslant K \tag{20}$$

and

$$\sum_{i=1}^{M} \tau_i^j f_A^c(k_i) = C_j, \quad 1 \leqslant j \leqslant K. \tag{21}$$

We come now to the main issue: the choice of the "distance" d. It seems natural to ask that

(i) d^2 be quadratic in the layering parameters, and
(ii) if two single-scale laminates differ only by a spatial rotation, their "distance" be proportional to the angle of the rotation.

The first property is desirable because it makes the minimization of Eq. (19) a quadratic optimization. The second reflects our viewpoint that a small rotation is a minor change of the structure, though it involves dramatic changes in the individual layer thicknesses.

Condition (ii) is very restrictive. For example the l^2 distance

$$\|\tau - \tau'\|_{l^2} = \left[\sum_{i=1}^{M} (\tau_i - \tau_i')^2 \right]^{1/2}$$

does not have this property. In fact, working in two space dimensions with an even number of layering directions $\{k_i\}$ equispaced on the unit half-circle, consider the choice $\tau_i = c$ if i is even and $\tau_i = 0$ if i is odd. If $\tau_{i+1}' = \tau_i$ then τ' corresponds to a rotation of τ by a small angle, but the distance between them is huge. Thus the l^2 distance is not an appropriate choice for d.

In fact, condition (ii) is too restrictive. There seems to be no distance d satisfying both (i) and (ii). However, we obtained good numerical results using

$$d(\tau, \tau') = \|F * (\tau - \tau')\|_{l^2}, \tag{22}$$

where $F*$ denotes a discrete convolution filter given by

$$(F * \tau)_i = \frac{1}{2r+1} \sum_{j=-r}^{r} \tau_{i+j} \tag{23}$$

and r is a fixed parameter (the bandwidth of the filter). Here we use the convention that the indices of τ are extended cyclically ($\tau_0 = \tau_M, \tau_{M+1} = \tau_1$, etc.). The parameter r must be reasonably large, to avoid the difficulties associated with the l^2 norm; however $2r+1$ must be below M, since when $2r+1 = M$ the convolution $F * \tau$ sees only the volume fraction $\sum \tau_i$.

Fig. 3 shows the performance of this scheme. Working in two space dimensions, we used $M = 51$ layering directions, equispaced on the unit half-circle. For the initial (continuously varying) Hooke's law we took C to

be a function of $x_1 \in [0,1]$, interpolating linearly between

- at $x_1 = 0$: the isotropic law with Lamé moduli $\lambda = .4166$ and $\mu = 0.4166$ (corresponding to Young's modulus $E = 2$ and Poisson's ratio $\nu = .2$ in plane stress), and
- at $x_1 = 1$: the orthotropic law associated with a two-layer single-scale laminate, using $\tau_1 = 2$ when the layer normal has angle $\pi/2$ and $\tau_2 = .5$ when the layer normal has angle 0.

The underlying material A was also chosen isotropic, with Lamé moduli $\lambda = .476$ and $\nu = .357$ (corresponding to Young's modulus $E = 1$ and Poisson's ratio $\nu = .4$ in plane stress).

We discretized the interval $0 \leqslant x_1 \leqslant 1$ using 10 equispaced nodes. Since the isotropic and orthotropic laws are both associated with single-scale laminates, preprocessing by the method of Section 4.1 is not necessary. But it is interesting to see what such preprocessing gives, since it reveals the character of the selections made by our semidefinite program (17). The results are shown in the top row of Fig. 3. The dependence is continuous in x_1, but the semidefinite program uses many layering directions (favoring uniformity).

The bottom row of Fig. 3 shows the result of minimizing Eq. (19) subject to Eqs. (20) and (21), when the distance d is given by Eqs. (22) and (23) with $r = 15$. (Recall that $M = 51$, so $(2r+1)/M \approx 3/5$.) The resulting structures depend continuously on x_1, and they also use relatively few layers. Interestingly, the layers in the rightmost figure are active (even dominant) in all simplified microstructures. This is true even at $x_1 = 0$ (Fig. 3(e)), where the Hooke's law is isotropic. Roughly: the minimization of Eq. (19) tends to reinforce the orthotropic microstructure in its diagonal directions. This is of course very different from the outcome of Section 4.2, where maximization of τ_l produced a triangular lattice.

The approach presented in this section is not limited to the case when C depends only on x_1. Indeed, the extension to more general spatial dependence is obvious. The associated quadratic program is rather large, because it involves KM variables where K is the number of spatial nodes and M is the number of layering directions. However, its structure is relatively sparse, since two nodes interact directly only if they are neighbors.

5. Analysis of the single-scale laminates

This section proves the Superposition and Optimality Principles, and discusses the connection between single-scale laminates and sequential laminates. We shall assume some familiarity with homogenization and optimal design, at the level of Allaire (2002).

Recall from Section 3.2 that a single-scale laminate is a porous composite made from a fixed elastic material A. Its microstructure consists of regularly spaced layers of thickness θt_i oriented normal to direction k_i, $1 \leqslant i \leqslant p$. Its local Hooke's law is thus of the form $\chi(y)A$ where χ takes only the values 0 and 1, and

$$\chi = \left(\sum_{i=1}^{p} \chi_i \right) - g^{(\mathrm{ov})}, \tag{24}$$

where χ_i is the characteristic function of the ith family of layers (a periodic function of $y \cdot k_i$, taking only the values 0 and 1, with average value θt_i) and $g^{(\mathrm{ov})}$ is supported in the region where the layers overlap (with $0 \leqslant g^{(\mathrm{ov})} \leqslant p$).

If the layering directions are rational then the structure is periodic, with a (possibly large) period cell. The general case can be approximated by such structures, so periodic homogenization is sufficient for proving theorems about the effective behavior. Moreover, since homogenization is a scale-invariant theory, there is no loss of generality in rescaling the structure so the unit cell is $Y = [0,1]^N$. We shall work throughout this section in these rescaled variables.

In discussing the Hooke's law of a single-scale laminate, our starting point is the familiar variational principle

$$\langle C_p^{(\mathrm{s})} \xi, \xi \rangle = \inf_{\Phi \in H^1_{\#}} \int \langle \chi(y) A(\xi + e(\Phi)), \xi + e(\Phi) \rangle \, \mathrm{d}y, \tag{25}$$

where the integral is over the period cell $Y=[0,1]^N$ and χ has the form (24). Here, and throughout this section, $H^1_\#$ denotes the class of Y-periodic H^1 functions.

5.1. The Superposition Principle

We shall prove upper and lower bounds that agree to leading order in volume fraction.

5.1.1. The lower bound

The primal variational principle (25) characterizes $\langle C_p^{(s)}\xi,\xi\rangle$ by a minimization over kinematically admissible periodic strain fields. For the lower bound, however, it is more convenient to work with its convex dual—a maximization over statically admissible periodic stress fields. We briefly review its well-known derivation, as an application of convex duality. Starting from Eq. (25) we have

$$\langle C_p^{(s)}\xi,\xi\rangle = \inf_{\Phi\in H^1_\#}\sup_{\sigma(y)}\int 2\langle\sigma,\xi+e(\Phi)\rangle-\langle(\chi(y)A)^{-1}\sigma,\sigma\rangle\,\mathrm{d}y,$$

where σ ranges over periodic "stress fields" that vanish where $\chi=0$. A standard duality theorem permits us to interchange the inf and sup, leading to

$$\begin{aligned}\langle C_p^{(s)}\xi,\xi\rangle &= \sup_{\sigma}\inf_{\Phi\in H^1_\#}\int 2\langle\sigma,\xi+e(\Phi)\rangle-\langle(\chi(y)A)^{-1}\sigma,\sigma\rangle\,\mathrm{d}y\\ &= \sup_{\operatorname{div}\sigma=0} 2\langle\bar\sigma,\xi\rangle-\fint_Y\langle(\chi(y)A)^{-1}\sigma,\sigma\rangle\,\mathrm{d}y.\end{aligned}$$

where $\bar\sigma$ denotes the average of σ. Recall that to be admissible for this dual variational principle, σ should be a periodic, symmetric-matrix-valued function that vanishes on the "holes" (where $\chi=0$). The constraint $\operatorname{div}\sigma=0$ is of course understood in the "weak sense:" σ must be divergence-free where there is material, and its normal traction $\sigma\cdot n$ must vanish at the boundaries of all holes.

We apply this with a "stress field" of the form

$$\sigma=\sum_{i=1}^p\chi_i(y)\sigma_i,$$

where χ_i is the characteristic function of the layers with normal k_i and σ_i is a (constant) element of $W(k_i)$. This choice is admissible, because each term $\chi_i(y)\sigma_i$ is admissible. To see why, we note (fixing i) that the condition $\sigma_i\in W(k_i)$ is equivalent to $\sigma_i\cdot k_i=0$. Thus the piecewise-constant test field $\chi_i(y)\sigma_i$ is periodic and weakly divergence free, and it vanishes where there is no material. Our stress field σ has mean

$$\bar\sigma=\theta\sum_{i=1}^p t_i\sigma_i+\mathcal{O}(\theta^2)$$

since the region where the layers overlap has volume fraction of order θ^2. We conclude from the dual variational principle that

$$\langle C_p^{(s)}\xi,\xi\rangle\geqslant 2\theta\sum_{i=1}^p t_i\langle\sigma_i,\xi\rangle-\theta\sum_{i=1}^p t_i\langle A^{-1}\sigma_i,\sigma_i\rangle+\mathcal{O}(\theta^2) \tag{26}$$

for any choice of $\sigma_i\in W(k_i)$.

We now choose the σ_i to maximize the order-θ terms on the right-hand side of Eq. (26). The optimality condition says that for each i, $2\theta t_i\xi-2\theta t_iA^{-1}\sigma_i$ is orthogonal to $W(k_i)$. Since $2\theta t_i\neq 0$, we conclude that $\{\sigma_i\}_{i=1}^p$ are optimal precisely when

$$\xi-A^{-1}\sigma_i\in V(k_i)\quad\text{for each } i. \tag{27}$$

In fact, the optimal σ_i can be given explicitly:

$$\sigma_i=A^{1/2}\Pi_{A^{-1/2}W(k_i)}A^{1/2}\xi=f_A^{\mathrm{c}}(k_i)\xi \tag{28}$$

using the notation introduced in Section 3.1. To justify Eq. (28), we need only show that this choice of σ_i satisfies Eq. (27). Recall from Eq. (4) that the space of $N \times N$ symmetric tensors has the orthogonal decomposition $A^{1/2}V(k_i) \oplus A^{-1/2}W(k_i)$. So $A^{1/2}\xi$ can be written uniquely as

$$A^{1/2}\xi = A^{1/2}\eta_i + A^{-1/2}\sigma_i$$

with $\eta_i \in V(k_i)$ and $\sigma_i \in W(k_i)$. Clearly these σ_i satisfy Eq. (27). Since $A^{-1/2}\sigma_i = \Pi_{A^{-1/2}W(k_i)}A^{1/2}\xi$ by definition, we have demonstrated Eq. (28).

Finally we evaluate the lower bound Eq. (26) at the optimal σ_i. Taking the inner product of Eq. (27) with σ_i gives

$$\langle A^{-1}\sigma_i, \sigma_i\rangle = \langle \sigma_i, \xi\rangle.$$

Therefore, the order-θ terms on the right-hand side of Eq. (26) reduce to $\theta\sum_{i=1}^{p} t_i\langle\sigma_i, \xi\rangle$. Replacing σ_i by its characterization (28), we conclude that

$$\langle C_p^{(s)}\xi, \xi\rangle \geqslant \theta \sum_{i=1}^{p} t_i \langle f_A^c(k_i)\xi, \xi\rangle + \mathcal{O}(\theta^2)$$

or in other words

$$C_p^{(s)} \geqslant \theta \sum_{i=1}^{p} t_i f_A^c(k_i) + \mathcal{O}(\theta^2). \tag{29}$$

This is the desired lower bound.

5.1.2. The upper bound

Our proof of the matching upper bound uses the Hashin–Shtrikman variational principle. To make the discussion self-contained, we start by reviewing its derivation. Starting from Eq. (25), we add and subtract the "reference energy" $\langle A(\xi + e(\Phi)), \xi + e(\Phi)\rangle$ to get

$$\begin{aligned}\langle C_p^{(s)}\xi, \xi\rangle = &\inf_{\Phi\in H^1_{\#}} \int \langle A(\xi + e(\Phi)), \xi + e(\Phi)\rangle \,\mathrm{d}y \\ &- \int (1 - \chi(y))\langle A(\xi + e(\Phi)), \xi + e(\Phi)\rangle \,\mathrm{d}y.\end{aligned} \tag{30}$$

For any (constant) $\eta \in \mathscr{M}_N$ we have

$$\langle A(\xi + e(\Phi)), \xi + e(\Phi)\rangle \geqslant 2\langle \eta, \xi + e(\Phi)\rangle - \langle A^{-1}\eta, \eta\rangle.$$

Substituting this into Eq. (30), we conclude that for any $\eta \in \mathscr{M}_N$,

$$\begin{aligned}\langle C_p^{(s)}\xi, \xi\rangle \leqslant &\inf_{\Phi\in H^1_{\#}} \int_Y \langle A(\xi + e(\Phi)), \xi + e(\Phi)\rangle \,\mathrm{d}y \\ &- \int 2(1 - \chi(y))\langle \eta, \xi + e(\Phi)\rangle - (1 - \chi(y))\langle A^{-1}\eta, \eta\rangle \,\mathrm{d}y.\end{aligned}$$

Integrating all terms that do not involve $e(\Phi)$, writing

$$\Theta = \int \chi(y)\,\mathrm{d}y = \theta + \mathcal{O}(\theta^2) \tag{31}$$

for the exact volume fraction of the composite, and using the fact that $e(\Phi)$ has mean value 0, we conclude that

$$\langle C_p^{(s)}\xi, \xi\rangle \leqslant \langle A\xi, \xi\rangle + (1 - \Theta)\langle A^{-1}\eta, \eta\rangle - 2(1 - \Theta)\langle \eta, \xi\rangle + I(\eta), \tag{32}$$

where

$$I(\eta) = \inf_{\Phi\in H^1_{\#}} \int \langle Ae(\Phi), e(\Phi)\rangle + 2\chi(y)\langle \eta, e(\Phi)\rangle \,\mathrm{d}y. \tag{33}$$

We can express $I(\eta)$ in terms of the Fourier transform of χ as follows. By Parseval's theorem,

$$I(\eta) = \inf_{\Phi \in H^1_{\#}} \sum_{k \in \mathbb{Z}^N \setminus \{0\}} \langle A\widehat{e(\Phi)}(k), \overline{\widehat{e(\Phi)}(k)} \rangle + 2\widehat{\chi}(k)\langle \eta, \overline{\widehat{e(\Phi)}(k)} \rangle.$$

Now, $\Phi \in H^1_{\#}(Y)$ is equivalent to $\widehat{e(\Phi)}(k) \in V(k)$ for each $k \in \mathbb{Z}^N \setminus \{0\}$ and $\widehat{e(\Phi)}(0) = 0$. (To keep the notation simple, we do not distinguish between $V(k)$ and its complexification.) The minimization over Φ can be done separately at each frequency: introducing the notation $e_k := \widehat{e(\Phi)}(k)$, we have

$$\begin{aligned} I(\eta) &= \sum_{k \in \mathbb{Z}^N \setminus \{0\}} \inf_{e_k \in V(k)} \langle Ae_k, \overline{e_k} \rangle + 2\widehat{\chi}(k)\langle \eta, \overline{e_k} \rangle \\ &= \sum_{k \in \mathbb{Z}^N \setminus \{0\}} \inf_{e_k \in V(k)} \langle A^{1/2}e_k, A^{1/2}\overline{e_k} \rangle + 2\widehat{\chi}(k)\langle A^{-1/2}\eta, A^{1/2}\overline{e_k} \rangle \\ &= \sum_{k \in \mathbb{Z}^N \setminus \{0\}} \inf_{\varphi_k \in V(k)} \{|A^{1/2}e_k + \widehat{\chi}(k)A^{-1/2}\eta|^2 - |\widehat{\chi}(k)|^2 |A^{-1/2}\eta|^2\}. \end{aligned}$$

The optimal choice of e_k is now clear: it is

$$e_k = -A^{-1/2}\Pi_{A^{1/2}V(k)}\widehat{\chi}(k)A^{-1/2}\eta$$

and substitution gives the value of $I(\eta)$:

$$I(\eta) = \sum_{k \in \mathbb{Z}^N \setminus \{0\}} |\widehat{\chi}(k)|^2 (|\Pi_{A^{-1/2}W(k)}A^{-1/2}\eta|^2 - |A^{-1/2}\eta|^2).$$

This can be expressed more compactly using the notation introduced in Section 3.1

$$I(\eta) = -\sum_{k \in \mathbb{Z}^N \setminus \{0\}} |\widehat{\chi}(k)|^2 \langle f_A(k)\eta, \eta \rangle,$$

with $f_A(k)\xi = A^{-1/2}\Pi_{A^{1/2}V(k)}A^{-1/2}\xi$. Thus the Hashin–Shtrikman bound (32) says

$$\langle C_p^{(s)}\xi, \xi \rangle \leqslant \langle A\xi, \xi \rangle + (1-\Theta)\langle A^{-1}\eta, \eta \rangle - 2(1-\Theta)\langle \eta, \xi \rangle - \sum_{k \in \mathbb{Z}^N \setminus \{0\}} |\widehat{\chi}(k)|^2 \langle f_A(k)\eta, \eta \rangle.$$

for any $\eta \in \mathscr{M}_N$. We could optimize over η, but it isn't necessary. Rather, we simply take $\eta = A\xi$. This gives

$$\langle C_p^{(s)}\xi, \xi \rangle \leqslant \Theta\langle A\xi, \xi \rangle - \sum_{k \in \mathbb{Z}^N \setminus \{0\}} |\widehat{\chi}(k)|^2 \langle f_A(k)A\xi, A\xi \rangle. \tag{34}$$

We have not yet used the hypothesis that the microstructure is a single-scale laminate: Eq. (34) applies to any porous composite made from the basic material A.

For a single-scale laminate we can go further: we shall show that

$$\sum_{k \in \mathbb{Z}^N \setminus \{0\}} |\widehat{\chi}(k)|^2 \langle f_A(k)A\xi, A\xi \rangle = \theta \sum_{i=1}^{p} t_i \langle f_A(k_i)A\xi, A\xi \rangle + \mathscr{O}(\theta^2). \tag{35}$$

Indeed, by Eq. (24) the left-hand side of Eq. (35) is equal to

$$\sum_{k \in \mathbb{Z}^N \setminus \{0\}} \left| \sum_{i=1}^{p} \widehat{\chi}_i(k) - \widehat{g^{(ov)}}(k) \right|^2 \langle f_A(k)A\xi, A\xi \rangle. \tag{36}$$

Since $\chi_i(y)$ is a function of $k_i \cdot y$, its Fourier transform $\widehat{\chi}_i(k)$ vanishes unless $k \| k_i$. Since the layering directions $\{k_i\}$ are assumed to be distinct, it follows that for $i \neq j$ we have:

$$\widehat{\chi}_i(k)\overline{\widehat{\chi}_j(k)} = 0 \quad \text{for all } k.$$

Therefore Eq. (36) equals

$$\sum_{k\in\mathbb{Z}^N\setminus\{0\}}\left[\sum_{i=1}^{p}(|\widehat{\chi_i}(k)|^2-2\widehat{\chi_i}(k)\cdot\overline{\widehat{g^{(\mathrm{ov})}}(k)})+|\widehat{g^{(\mathrm{ov})}}(k)|^2\right]\langle f_A(k)A\xi,A\xi\rangle.$$

The terms involving $g^{(\mathrm{ov})}$ are of order $\mathcal{O}(\theta^2)$. To see this, observe using Eq. (9) that

$$|\langle f_A(k)A\xi,A\xi\rangle|=|\langle\Pi_{A^{1/2}V(k)}A^{1/2}\xi,A^{1/2}\xi\rangle|\leqslant\|A^{1/2}\xi\|^2;$$

in particular it is uniformly bounded, independent of k. Since the support of $g^{(\mathrm{ov})}$ has volume of order θ^2 and $g^{(\mathrm{ov})}$ is pointwise less than or equal to p, an application of Plancherel's theorem gives

$$\sum_{k\in\mathbb{Z}^N\setminus\{0\}}|\widehat{g^{(\mathrm{ov})}}(k)|^2=\mathcal{O}(\theta^2).$$

Similarly,

$$\begin{aligned}\sum_{k\in\mathbb{Z}^N\setminus\{0\}}\widehat{\chi_i}(k)\cdot\overline{\widehat{g^{(\mathrm{ov})}}(k)}&=\sum_{k\in\mathbb{Z}^N}\widehat{\chi_i}(k)\cdot\overline{\widehat{g^{(\mathrm{ov})}}(k)}-\widehat{\chi_i}(0)\widehat{g^{(\mathrm{ov})}}(0)\\&=\int\chi_i(y)g^{(\mathrm{ov})}(y)\,\mathrm{d}y-\mathcal{O}(\theta^3)=\mathcal{O}(\theta^2),\end{aligned}$$

since $\chi_i(y)g^{(\mathrm{ov})}(y)\leqslant g^{(\mathrm{ov})}(y)$ and $\int g^{(\mathrm{ov})}(y)\,\mathrm{d}y=\mathcal{O}(\theta^2)$. Thus Eq. (36) equals

$$\sum_{k\in\mathbb{Z}^N\setminus\{0\}}\sum_{i=1}^{p}|\widehat{\chi_i}(k)|^2\langle f_A(k)A\xi,A\xi\rangle+\mathcal{O}(\theta^2)\tag{37}$$

as asserted.

To evaluate Eq. (37), we recall that for each i, $\chi_i(y)$ is a periodic function of y taking only values 0 and 1, with average value $\overline{\chi}_i=t_i\theta$. Therefore, by Plancherel's theorem,

$$\sum_{k\in\mathbb{Z}^N\setminus\{0\}}|\widehat{\chi_i}(k)|^2=\int|\chi_i-\overline{\chi}_i|^2\,\mathrm{d}y=t_i\theta(1-t_i\theta).$$

Substituting this into Eq. (37) and summing over i, we obtain the desired formula (35) for the nonlocal term in the Hashin–Shtrikman bound.

Wrapping up: when the microstructure is a single-rank laminate, the total volume fraction is $\Theta=\theta\sum_{i=1}^{p}t_i+\mathcal{O}(\theta^2)$ and the upper bound (34) reduces to via Eq. (35) to

$$\langle C_p^{(\mathrm{s})}\xi,\xi\rangle\leqslant\theta\sum_{i=1}^{p}t_i[\langle A\xi,\xi\rangle-\langle f_A(k_i)A\xi,A\xi\rangle]+\mathcal{O}(\theta^2).$$

Recalling from Eq. (8) that $A-Af_A(k)A=f_A^{\mathrm{c}}(k)$, we have shown that

$$C_p^{(\mathrm{s})}\leqslant\theta\sum_{i=1}^{p}t_if_A^{\mathrm{c}}(k_i)+\mathcal{O}(\theta^2),\tag{38}$$

in the sense of quadratic forms. This is the desired upper bound. Taken together, Eq. (29) and (38) prove the validity of the Superposition Principle.

Remark 5.1. Stresses in the layers: Since the lower and upper bounds match at leading order, each of the inequalities that led to the bounds must actually be an equality at leading order. In particular, our lower bound (26) becomes

$$\langle C_p^{(\mathrm{s})}\xi,\xi\rangle=2\theta\sum_{i=1}^{p}t_i\langle\sigma_i,\xi\rangle-\theta\sum_{i=1}^{p}t_i\langle A^{-1}\sigma_i,\sigma_i\rangle+\mathcal{O}(\theta^2)$$

when

$$\sigma_i = A^{1/2}\Pi_{A^{-1/2}W(k_i)}A^{1/2}\xi.$$

It follows that σ_i is (to leading order) the *stress in the* ith *family* of layers.

Remark 5.2. Comparing the proofs of the lower and upper bounds: We proved the lower bound in Section 5.1.1 by applying the dual variational principle to a superposition of admissible piecewise-constant "stress fields" $\chi_i(y)\sigma_i$. The argument worked because the supports of these "stress fields" were almost disjoint: $\sigma = \sum_i \chi_i(y)\sigma_i$ vanishes where there is no material and equals σ_i in the ith family of layers, except in the regions where layers overlap (whose volume is $\mathcal{O}(\theta^2)$). It is natural to ask whether the upper bound can be proved by a similar argument. The answer, we think, is no. The reason is that the analogous piecewise-constant "strain fields" for a layered composite do not vanish in the void. It is of course possible to consider a superposition of (kinematically admissible) piecewise-constant strain fields associated with the different layering directions; however they would interact, making an argument parallel to Section 5.1.1 impossible.

5.2. Proof of the Optimality Principle

The Optimality Principle is the analogue for single-scale laminates of a well-known result from Avellaneda (1987). That work considered two-component composites made from two well-ordered, nondegenerate materials with Hooke's laws $B<A$. It showed the "optimality" of sequential laminates (for problems where stiffness is preferred), by proving that if C is the Hooke's law of any composite then there is a sequential laminate—made from the same two materials, using the same volume fractions—whose Hooke's law $C_+^{(l)}$ satisfies $C \leqslant C_+^{(l)}$. The proof had two main ingredients: the Hashin–Shtrikman upper bound, and an exact formula for the Hooke's law of a sequential laminate.

Our Optimality Principle follows (at least formally) from Avellaneda's result, by: (i) passing to the limit $B \to 0$, then (ii) using the results in Section 5.3, which relate the Hooke's laws of single-scale and sequential laminates. But it is simpler and much more direct to give a self-contained proof, applying the strategy of Avellaneda's argument directly to the setting of single-scale laminates. Since the main ingredients—the Hashin–Shtrikman bound and a formula for the Hooke's law—are already in hand, the proof is quite short.

We start from the Hashin–Shtrikman upper bound Eq. (34), which can be written as

$$C \leqslant \Theta A - \sum_{k\in\mathbb{Z}^N\setminus\{0\}} |\widehat{\chi}(k)|^2 A f_A(k) A. \tag{39}$$

Recall that we proved this for *any* porous composite, not just single-rank laminates. The function χ was the characteristic function of the microstructure (in other words, the local Hooke's law was $\chi(y)A$) and Θ was the volume fraction where $\chi = 1$. By Plancherel,

$$\sum_{k\in\mathbb{Z}^N\setminus\{0\}} |\widehat{\chi}(k)|^2 = \int |\chi - \Theta|^2 \,\mathrm{d}y = \Theta(1-\Theta);$$

and by Eq. (8) we have $A - A f_A(k) A = f_A^{\mathrm{c}}(k)$, so Eq. (39) can be written

$$C \leqslant \Theta \sum_{k\in\mathbb{Z}^N\setminus\{0\}} t_k f_A^{\mathrm{c}}(k) + \mathcal{O}(\Theta^2)$$

with $t_k = |\widehat{\chi}(k)|^2/\Theta(1-\Theta)$. Since $\sum t_k = 1$, the sum on the right is a convex combination of the degenerate Hooke's laws $\{f_A^{\mathrm{c}}(k)\}$. In other words, it lies in the closed convex hull of $\{f_A^{\mathrm{c}}(k)\}_{k\in\mathbb{S}^{N-1}}$ (recall that $f_A^{\mathrm{c}}(k)$ depends only on $k/|k|$). By Caratheodory's theorem, every point in this set is a convex combination of finitely many extreme points. Therefore, there exist positive numbers $t'_1,\ldots,t'_p$ (with $\sum t'_i = 1$) and unit vectors $k'_1,\ldots,k'_p$ such that

$$\sum_{k\in\mathbb{Z}^N\setminus\{0\}} t_k f_A^{\mathrm{c}}(k) = \sum_{i=1}^{p} t'_i f_A^{\mathrm{c}}(k'_i), \tag{40}$$

whence

$$C \leqslant \Theta \sum_{i=1}^{p} t_i' f_A^{\mathrm{c}}(k_i') + \mathcal{O}(\Theta^2).$$

This proves the Optimality Principle (12): C is, to leading order, less than or equal to the Hooke's law

$$C_+^{(\mathrm{s})} = \Theta \sum_{i=1}^{p} t_i' f_A^{\mathrm{c}}(k_i')$$

of a single-scale laminate made from the same material A using the same volume fraction Θ.

Remark 5.3. What if compliance is preferred? The Optimality Principle says that for any porous composite C, there is single-scale laminate with the same volume fraction that's stiffer (to leading order) than C. Is there also a single-scale laminate that's more compliant? We think not. (For example, if the base material A is isotropic then there is only *one* isotropic composite C that's achievable as a single-scale laminate; it is, by the Optimality Principle, the stiffest isotropic high-porosity composite achievable by mixing A with void.) However, if C is nondegenerate (that is, if $C>0$), then there are plenty of *single-scale composites* with the same volume fraction that are more compliant. To achieve this, let θ be the volume fraction of material in C, and consider *any* single-scale laminate with the same volume fraction; suppose its Hooke's law is $C_{\mathrm{ssl}} = \theta \sum_i t_i f_A^{\mathrm{c}}(k_i)$. If C is nondegenerate then we can choose $\alpha>0$ small enough that $\alpha C_{\mathrm{ssl}} \leqslant C$. Thus there is a single-scale laminate with volume fraction $\alpha\theta$ that is more compliant than C. Now, for porous composites it is always easy to "waste" material—it suffices to include, as part of the unit cell, a region of material that's disconnected from the rest of the structure. By starting from the single-scale laminate with volume fraction $\alpha\theta$ then "wasting" volume fraction $(1-\alpha\theta)$, we obtain a porous composite with volume fraction θ that's more compliant than C. It is not a single-scale laminate, but it is certainly a porous composite with a relatively simple single-scale microstructure.

5.3. Single-scale and sequential laminates

The optimal design literature has devoted a lot of attention to sequential laminates, because for problems where stiffness is preferred an optimal microstructure can always be found in this class.

Our single-scale laminates can be viewed as "sequential laminates without the separation of scales." Indeed, the optimal two-component sequential laminates considered in the optimal design literature mix two well-ordered materials with Hooke's laws $B<A$. We shall show that when $B=0$, the Hooke's law of a sequential laminate agrees to leading order with the Hooke's law of the associated single-scale laminate. Thus the separation of scales implicit in sequential lamination is unimportant in the high-porosity limit.

A single-scale laminate has layers of thickness θt_i oriented normal to k_i, $1 \leqslant i \leqslant p$. Here θ is a scale factor (the volume fraction, to leading order) and the relative thicknesses are normalized by $\sum_{i=1}^{p} t_i = 1$. We define a corresponding sequential laminate with Hooke's law $C_p^{(\mathrm{l})}$ by the following iterative procedure: Fixing two Hooke's laws $B<A$,

- let $C_1^{(\mathrm{l})}$ be the Hooke's law of the composite obtained by mixing A and B in layers normal to k_1, using volume fraction θt_1 of A;
- then for $2 \leqslant i \leqslant p$, let $C_i^{(\mathrm{l})}$ be the Hooke's law of the composite obtained by mixing A with $C_{i-1}^{(\mathrm{l})}$ in layers normal to k_i, using volume fraction θt_i of A and $(1-\theta t_i)$ of $C_{i-1}^{(\mathrm{l})}$.

The Hooke's laws $C_i^{(\mathrm{l})}$ have simple, explicit formulas. The initial step gives

$$(1-\theta t_1)(C_1^{(\mathrm{l})^{-1}} - A^{-1})^{-1} = (B^{-1} - A^{-1})^{-1} + \theta t_1 f_A^{\mathrm{c}}(k_1). \tag{41}$$

(This is Eq. (2.70) of Allaire (2002); the focus there is on isotropic A, but as shown for example in Allaire and Kohn (1993a) the formula is also valid when A is anisotropic. The proof resembles the calculation we did in

Section 3.1.) The subsequent steps give

$$\left[\prod_{i=1}^{p}(1-\theta t_i)\right](C_p^{(l)^{-1}}-A^{-1})^{-1}=(B^{-1}-A^{-1})^{-1}+\theta\sum_{i=1}^{p}l_i f_A^c(k_i), \tag{42}$$

where the parameters l_i are defined by

$$l_i=t_i\prod_{j=1}^{i-1}(1-\theta t_j). \tag{43}$$

Note that the microstructure associated with $C_p^{(l)}$ has overall volume fraction Θ of material A, where

$$\Theta=1-\left[\prod_{i=1}^{p}(1-\theta t_i)\right]. \tag{44}$$

(Eq. (42) is equivalent to Allaire's equation (2.73); our parameters $\{l_i\}$ correspond to Allaire's parameters $\{m_i\}$ by $m_i=\theta l_i/\Theta$.) Our goal is to show that in the limit $B\to 0$, $C_p^{(l)}$ agrees (to leading order in θ) with the Hooke's law of a single-scale laminate.

To warm up, let us start with the special case $p=1$. Eq. (41) gives the Hooke's law of a layered mixture of A and B in volume fractions $1-\theta t_1$ and θt_1, respectively. We claim that it reduces, when $B\to 0$, to the result proved in Section 3.1:

$$C=\theta t_1 f_A^c(k_1). \tag{45}$$

To see why, recall that $f_A^c(k)=A^{1/2}\Pi_{A^{-1/2}W(k)}A^{1/2}$. To simplify notation, we replace θt_1 by θ and write k rather than k_1. Then Eq. (41) is equivalent to

$$(1-\theta)([A^{-1/2}C_1^{(l)}A^{-1/2}]^{-1}-I)^{-1}=([A^{-1/2}BA^{-1/2}]^{-1}-I)^{-1}+\theta\Pi_{A^{-1/2}W(k)} \tag{46}$$

and Eq. (45) is equivalent to

$$A^{-1/2}CA^{-1/2}=\theta\Pi_{A^{-1/2}W(k)}. \tag{47}$$

As $B\to 0$, the right-hand side of Eq. (46) reduces to $\theta\Pi_{A^{-1/2}W(k)}$. Now, if Π_X is orthogonal projection on any subspace X we have the operator identity

$$(1-\theta)([\theta\Pi_X]^{-1}-I)^{-1}=\theta\Pi_X \tag{48}$$

since both sides vanish on the orthogonal complement of X (where $\Pi_X=0$, so $\Pi_X^{-1}=\infty$), while both sides act as multiplication by $(1-\theta)(\theta^{-1}-1)^{-1}=\theta$ on X. We conclude that when $B\to 0$, the left-hand side of (46) reduces to the left-hand side of (48) with $X=A^{-1/2}W(k)$. It follows that $C=\lim_{B\to 0}C_1^{(l)}$ satisfies (47), as asserted. Note that this is *not* a low-volume-fraction result; it holds for any value of θ, $0<\theta<1$.

The argument for general p is similar, however, we will need to use the smallness of θ at the very end. Our goal is to show that in the limit $B\to 0$, the Hooke's law $C_p^{(l)}$ of the sequential laminate agrees to leading order with the Hooke's law $C_p^{(s)}$ of the associated single-scale laminate. Using the form of $f_A^c(k)$, the definition (42) of $C_p^{(l)}$ is equivalent to

$$(1-\Theta)([A^{-1/2}C_p^{(l)}A^{-1/2}]^{-1}-I)^{-1}=([A^{-1/2}BA^{-1/2}]^{-1}-I)^{-1}+\theta\sum_{i=1}^{p}l_i\Pi_{A^{-1/2}W(k_i)}. \tag{49}$$

Similarly, the definition (11) of $C_p^{(s)}$ is equivalent to

$$A^{-1/2}C_p^{(s)}A^{-1/2}=\theta\sum_{i=1}^{p}t_i\Pi_{A^{-1/2}W(k_i)}+\mathcal{O}(\theta^2). \tag{50}$$

We note for later reference that

$$\Theta=\theta+\mathcal{O}(\theta^2)\quad\text{and}\quad l_i=t_i+\mathcal{O}(\theta) \tag{51}$$

as easy consequences of the definitions (43) and (44).

When $B \to 0$, the right-hand side of Eq. (49) reduces to θL where

$$L = \sum_{i=1}^{p} l_i \Pi_{A^{-1/2}W(k_i)}.$$

Note that L is a nonnegative, symmetric linear map. Its kernel is the orthogonal complement of

$$X = \text{linear span of } A^{-1/2}W(k_1), \ldots, A^{-1/2}W(k_p)$$

and its restriction to X is invertible. Writing

$$C = \lim_{B \to 0} C_p^{(l)}$$

we conclude that $A^{-1/2}CA^{-1/2}$ vanishes on the orthogonal complement of X, and

$$(1-\Theta)([A^{-1/2}CA^{-1/2}]^{-1} - I)^{-1} = \theta L \tag{52}$$

on X. Since the restriction of L to X is positive definite, it has an inverse $L^{-1} : X \to X$ (strictly speaking: L^{-1} is the *pseudoinverse* of L). Inverting both sides of Eq. (52), we have

$$[A^{-1/2}CA^{-1/2}]^{-1} - I = \frac{1-\Theta}{\theta} L^{-1}$$

as linear maps on X. Therefore,

$$[A^{-1/2}CA^{-1/2}]^{-1} = \frac{1-\Theta}{\theta} L^{-1}\left(I + \frac{\theta}{1-\Theta} L\right)$$

and inverting again gives

$$A^{-1/2}CA^{-1/2} = \frac{\theta}{1-\Theta} L\left(I + \frac{\theta}{1-\Theta} L\right)^{-1}.$$

In the low-volume-fraction regime, this becomes

$$A^{-1/2}CA^{-1/2} = \theta \sum_{i=1}^{p} t_i \Pi_{A^{-1/2}W(k_i)} + \mathcal{O}(\theta^2)$$

by Eq. (51). Comparing with Eq. (50), we see that C is, to leading order, the effective Hooke's law $C_p^{(s)}$ of the single-scale laminate.

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