OPTIMALITY CONDITIONS ON FIELDS IN MICROSTRUCTURES AND CONTROLLABLE DIFFERENTIAL SCHEMES

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Abstract. Optimal microstructures are layouts of several materials in the periodicity cell which attain the extreme value of the sum of energies, W, of several linearly independent homogeneous external fields (loadings). The extremal value of W can be found or estimated from below by using the sufficient conditions for the corresponding nonconvex variational problem. We describe an algorithm for constructing optimal isotropic three-dimensional microstructures that attain the sufficient conditions. The layouts are limits of geometrical sequences with infinitely many length scales and are nonunique. In contrast, the fields in the optimal structures are clearly defined by sufficient constraints that hold in each point. In the paper, we discuss a modified differential scheme that produces an optimal laminate while keeping the field in each point within the prescribed range.

As a first example, we describe fields in an optimal three-dimensional polycrystal. The sufficient constraints lead to non-compatible (not rank-one connected) fields in the disoriented fragments of the crystallite. The apparent contradiction of non-compatibility is resolved by using infinitely many length scales. This phenomenon is similar to the two-dimensional example of four non-compatible gradients Pedregal (1993); Tartar (1993); Nesi and Milton (1991).

A second example produces new optimal microstructures of three-dimensional three-material isotropic mixture. These structures are optimal in the range of parameters that is larger than the previously known range Milton (1981); Milton and Kohn (1988). The method is also applicable to more than three materials as well as to elastic, electromagnetic and other linear materials.

1. Introduction

This paper suggests an approach to building optimal composite structures. The approach is based on two principles. First, pointwise sufficient conditions for the fields in each phase of the composite are found by using translation bounds. Second, these conditions are incorporated into the differential scheme for building the composite which then produces optimal

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generalized microgeometry. The structures obtained in this way are infinite-rank laminates.

The problem of the G-closure boundary – the set of structures with extreme effective properties – has a long history. Optimal microstructures are traditionally found by a two-step procedure. First, one derives sufficient optimality conditions (translation bounds) for the energy. Second, one attempts to generate minimizing sequences of layouts which satisfy these conditions. A number of problems for two-material microstructures have been solved, see the books Cherkaev (2000); Milton (2002) and the references therein. However, for more complicated problems, such as the examples in this paper, a more formalized procedure for generating optimal microstructures is necessary. The conventional approach has been to make a clever guess of the basic microstructure with a few free design parameters and then to optimize with respect of these parameters. If one is lucky, the structure obtained by this process is optimal. Unfortunately for complex problems, it has not proven easy to make a good guess.

Our approach, although not fully free of guess, exploits formalized procedures. Specifically, we find the sufficient conditions for the fields in optimal microstructures. These conditions are used in the variant of the "differential scheme" to produce an of optimal microstructures; the optimality of the sequence is built into the procedure and is ensured at every differential step. Thus, the problem of optimal microstructures is formulated as an extremal problem with differential constraints.

2. The problem

2.1. **Statement.** Consider a periodic structure. The periodicity cell $\Omega = [0,1]^3 \subset R^3$ has unit measure and is subdivided into subsets Ω_i occupied by N materials with conductivity tensors K_i. Consider three separate conductivity equilibria, induced by the homogeneous external fields $e_1 \cdot (1,0,0)$, $e_2 \cdot (0,1,0)$, $e_3 \cdot (0,0,1)$ applied to the cell. If we denote $E = \mathrm{Diag}(e_1, e_2, e_3)$ then the three conductivity equations in the cell can be concisely expressed as

$$\nabla \cdot K \nabla u = 0, \ \langle \nabla u \rangle = E. \tag{1}$$

Here u is a three-dimensional vector function, ∇u is a 3×3 matrix with components $(\nabla u)_{ij} = \frac{\partial u_i}{\partial x_j}$ and $\nabla \cdot$ is the row-wise divergence operator which transforms a matrix into a vector, as

$$(\nabla \cdot A)_i = \sum_{j=1}^{3} \frac{\partial A_{ij}}{\partial x_j}, \quad i = 1,2,3.$$

The conductivity tensor K is defined to be K_i in Ω_i.

The sum of the three energies can be written as

$$W = \langle [K \nabla u, \nabla u] \rangle ; \tag{2}$$

where $[A,B]$ is the scalar product on square matrices, $[A,B]=\mathrm{Tr}A^TB$, and $\langle\cdot\rangle$ is the average over Ω. The energy W is equal to the energy of the homogenized material with the *effective conductivity* K_*

$$W=\left[K_*\langle\nabla u\rangle,\langle\nabla u\rangle\right]. \tag{3}$$

In this paper, we consider the following problem: for fixed e_i, minimize the energy W by choosing the layouts of the K_i, assuming that the areas of Ω_i (the volume fractions) are fixed: $|\Omega_i|=m_i$. In the rest of this section we recall the traditional method of solving this problem specifically as applied to our two examples of polycrystals and multi-material mixtures.

2.2. **Translation bounds and the fields in an optimal structure.**

The bound. The translation bound (see Cherkaev (2000); Milton (2002) and the references therein) restricts the energy, W, of a structure from below, thus providing a bound for its effective properties. The energy is bounded from below by the function $W_T\le W$ where

$$W_T=\max_{T\in\mathcal{T}}[D_T\langle\nabla u\rangle,\langle\nabla u\rangle];\quad \mathcal{T}=\{T:\ D_i-T\ge 0\ \forall i=1,...,N\}$$

and

$$D_T=\left(\sum_{i=1}^{N}m_i(D_i-T)^{-1}\right)^{-1}+T.$$

Here, the D_i and T are linear operators on 3×3 matrices. Specifically, $[D_iE,E]=\mathrm{Tr}(E^TK_iE)$ for $i=1,...,N$ and $[TE,E]$ is the quadratic invariant of the matrix E (see Cherkaev (2000) for the discussion of the structure of the translators)

$$[TE,E]=-\frac{t}{2}\left((\mathrm{Tr}E)^2-\mathrm{Tr}E^2\right)$$

– a constant times the sum of the three main 2×2 minors. Any structure with energy equal to W_T is called translation-optimal.

In the next calculation, we represent E by a nine-dimensional vector of its elements by stacking its rows,

$$E=(e_1\ 0\ 0\mid 0\ e_2\ 0\mid 0\ 0\ e_3)^T. \tag{4}$$

In this space, the tensors D_i are represented as 9×9 matrices. In particular, an isotropic conductivity tensor $K_i=k_iI_3$, where I_3 is the 3×3 identity matrix, is represented by the matrix $D_i=k_iI_9$, where I_9 is the 9×9 identity matrix. Furthermore, T is represented by the following 9×9 symmetric

matrix.

$$T(t) = -\left(\begin{array}{ccc|ccc|ccc} 0 & 0 & 0 & 0 & t & 0 & 0 & 0 & t \\ 0 & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 \\ \hline 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 \\ \hline 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 \\ t & 0 & 0 & 0 & t & 0 & 0 & 0 & 0 \end{array}\right) \tag{5}$$

The fields. The translation bound corresponds to certain constraints on the pointwise field $\nabla u(x)$ (see also Grabovsky (1996); Milton (2002)). The fields in the phases of a translation-optimal structure pointwise satisfy the equations

$$(D_i - T)E_i = RE_0, \quad R = \left(\sum_{p=1}^{N} m_p (D_p - T)^{-1}\right)^{-1} \qquad i = 1, \dots, N. \tag{6}$$

Besides this, the following integral constraint holds.

$$\sum_{p=1}^{N} m_p \int_{\Omega_p} E_p \, dx = E_0. \tag{7}$$

This is automatically satisfied when the fields E_i found from (6) are unique. The matrices $D_i - T$ are nonnegative definite. When these matrices are positive definite, the fields E_i are uniquely defined by a relation

$$E_i = (D_i - T)^{-1} R \, E_0; \tag{8}$$

matrix $(D_i - T)^{-1}R$ is positive. The second equation (7) is automatically satisfied in this case.

Nontrivial bounds correspond to the cases when the translator T is chosen so that one or several of the matrices $D_i - T$ degenerate. In this case, matrices $(D_i - T)^{-1}$ and R are redefined on the appropriate subspace. The fields E_i belong to some linear subspaces independently of E_0. Below, we list the possible degenerations.

(1) Assume that $D_k - T$ $(k \neq i)$ degenerates

$$D_k - T = Q_k \, Q_k^T \quad Q \in \mathbb{R}^{m_k \times n} \tag{9}$$

but $D_i - T$ does not. Then the right-hand side term R degenerates because the projection onto the orthogonal to Q subspace is zero. It assumes the form

$$R = Q_k \tilde{R} Q_k^T \tag{10}$$

where $\tilde{R} \in \mathbb{R}^{m_k \times m_k}$ is

$$\tilde{R} = \left(Q_k^T R^{-1} Q_k\right)^{-1}.$$

If several terms $D_{k_1} - T, \dots D_{k_s} - T$, $(k_1 \neq i, \dots k_s \neq i)$ degenerate, the right-hand side term R takes the form

$$R = \tilde{Q}\tilde{R}\tilde{Q}^T \tag{11}$$

where

$$\tilde{Q} = Q_{k_1} \dots Q_{k_s}. \tag{12}$$

The field E_i depends on the projection of E_0 onto the subspace $\tilde{Q}$,

$$(D_i - T)E_i = \tilde{Q}\tilde{R}(\tilde{Q}^T E_0) \tag{13}$$

(2) Assume that $D_i - T$ degenerates,

$$D_i - T = Q_i\, Q_i^T \quad Q \in \mathbb{R}^{m_i \times n} \tag{14}$$

but $D_k - T$ $(k \neq i)$ are positive definite. In this case, equation (6) does not uniquely define the field E_i. Its solution has the form

$$R\, E_0 = Q_i^T E_i + \alpha h, \quad Q_i^T h = 0 \tag{15}$$

where α is an arbitrary real function that can vary in Ω_i and h is a n-vector orthogonal to Q_i. Equation (7) constrains $\alpha = \alpha(x)$. The m_i-dimensional vector $Q_i^T E_i$ – a projection onto Q_i – depends on E_0 as

$$Q_i^T E_i = (Q_i^T Q_i)^{-1} Q_i^T R^{-1}\, E_0. \tag{16}$$

(3) Finally, assume that two matrices $D_i - T$ and $D_k - T$ $(k \neq i)$ degenerate as happens in the problem of an optimal polycrystal. The field E_i has the form (15), but the term $R\, E_0$ is decomposed as in (13). We obtain

$$Q_i^T E_i = (Q_i^T Q_i)^{-1} Q_i^T \tilde{Q}\tilde{R}(\tilde{Q}^T E_0). \tag{17}$$

The field $E_i = Q_i^T E_i + \alpha h$ is nonunique and depends only on the projection of E_0 onto a subspace $\tilde{Q}$.

2.3. **Examples: translation-optimal fields.** We illustrate the translation bound using two examples. First is the three-dimensional isotropic polycrystal of minimal conductivity. The structure was found in Avellaneda et al. (1988) and then discussed in Nesi and Milton (1991); Cherkaev (2000); Milton (2002). Here, we focus on the fields in optimal polycrystals. The second example is the problem of translation-optimal isotropic three-phase composites from several isotropic components. We refer to Cherkaev (2000); Milton (2002) for a history of this problem and further references. It is known, in particular, that translation-optimal structures exist only in a range of parameters: the fraction of the "best" material must be large enough. In the next section we find new translation-optimal structures with lower limit on the fraction of the best material.

Polycrystals. Consider a polycrystal – a composite from differently oriented fragments of an anisotropic material. Specifically, consider differently oriented transversally isotropic conducting materials such that two eigenvalues are equal and one differs. After normalization the equal eigenvalues are assumed to be one and the third eigenvalue to be $s \neq 1$. Assume that we mix three anisotropic materials with the same triplet of eigenvectors, but such that the eigenvalue s corresponds to a different eigenvector in each phase. Further, assume that the polycrystal is isotropic, and the three mixed materials enters with the same volume fraction 1/3. The extremal effective conductivity (lower bound) and the minimizing sequence was found in Avellaneda et al. (1988), see also Cherkaev (2000). Here we calculate fields in these translation-optimal structures, using the theory discussed above.

The matrices D_i are diagonal.

$$D_1 = \mathrm{Diag}(s\ 1\ 1 \mid s\ 1\ 1 \mid s\ 1\ 1),$$

$$D_2 = \mathrm{Diag}(1\ s\ 1 \mid 1\ s\ 1 \mid 1\ s\ 1),$$

$$D_3 = \mathrm{Diag}(1\ 1\ s \mid 1\ 1\ s \mid 1\ 1\ s).$$

The translator T used in this case is given by (5). The external fields are represented by the nine component of the diagonal 3×3-matrix E_0. Because we restrict to orthogonal nonzero external fields and diagonal conductivity tensors, one can show that it is sufficient to consider diagonal pointwise fields. Thus, we may project from the space of 9-vectors to the the first, fifth, and ninth components (see (5)).

The nontrivial bound can be found from the projection onto this three-dimensional subspace of the diagonal components of the fields and the corresponding projection of T. The projections, $\hat{D}_i$ and $\hat{T}$, of the D_i and T respectively, are

$$-\hat{T}(t) = \begin{pmatrix} 0 & t & t \\ t & 0 & t \\ t & t & 0 \end{pmatrix}, \quad \hat{D}_1 - \hat{T}(t) = \begin{pmatrix} 1 & t & t \\ t & s & t \\ t & t & 1 \end{pmatrix}, \tag{18}$$

$$\hat{D}_2 - \hat{T}(t) = \begin{pmatrix} 1 & t & t \\ t & s & t \\ t & t & 1 \end{pmatrix}, \quad \hat{D}_3 - \hat{T}(t) = \begin{pmatrix} 1 & t & t \\ t & 1 & t \\ t & t & s \end{pmatrix}. \tag{19}$$

Consider for definiteness the translation-optimal field E_1 in the fragments D_1. The extremal value t_0 of t that correspond to degenerations of all three matrices, is

$$t_0 = \frac{1}{4}\left(s - \sqrt{s(s+8)}\right).$$

The eigenvalues λ_k of $\hat{D}_1 - \hat{T}(t_0)$ are

$$\lambda_1 = 0, \quad \lambda_2 = \frac{1}{4}\sqrt{s(s+8)} - \frac{1}{4}s + 1, \quad \lambda_3 = \frac{5}{4}s - \frac{1}{4}\sqrt{s(s+8)} + 1$$

The eigenvectors $a_k^{(1)}$ are

$$a_1^{(1)} = \begin{pmatrix} \gamma_1 \\ 1 \\ 1 \end{pmatrix} \quad a_2^{(1)} = \begin{pmatrix} \gamma_2 \\ 1 \\ 1 \end{pmatrix} \quad a_3^{(1)} = \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$$

where

$$\gamma_1 = \frac{\sqrt{s^2+8s}-s}{2s} \quad \gamma_2 = 2\frac{\sqrt{s^2+8s}-s}{\sqrt{s^2+8s}-s+4}.$$

The eigenvalues of the other two phases are the same, and the eigenvectors are obtained by a corresponding permutation of $a_k^{(i)}$.

The fields in translation-optimal polycrystals are computed as in case 3 above. The fields E_1, E_2, E_3 in the differently oriented crystallites in the translation-optimal polycrystal are constrained as follows

$$\begin{aligned} E_1 &\in \{\tau \mathrm{Diag}(\gamma_1, 1, 1) : \tau \in \mathbb{R}\}, \\ E_2 &\in \{\tau \mathrm{Diag}(1, \gamma_1, 1) : \tau \in \mathbb{R}\}, \\ E_3 &\in \{\tau \mathrm{Diag}(1, 1, \gamma_1) : \tau \in \mathbb{R}\}. \end{aligned} \tag{20}$$

From this, one can derive the following equation for the effective conductivity $K_* = k_* I$ of a translation-optimal polycrystal.

$$k_* = -2t_0 = \frac{1}{2}\left(\sqrt{s(s+8)} - s\right).$$

In a translation optimal anisotropic crystallite, the field in each phase belongs to a given line. Notice that the only rank-one connections among the different lines lie at zero. This implies that there is no finite-rank optimal laminate that realizes the bound. However, the optimal structure exists and the apparent contradiction can be resolved, as we discuss in the next section. Optimal composite from isotropic components. Consider an isotropic N-material mixture of isotropic materials $K_i = k_i I_3$ where $k_i \in \mathbb{R}$ is an isotropic conductivity tensor; assume that the materials are ordered so that $0 < k_1 < \cdots < k_N$. Assume also that the external fields are orthogonal. Let us find the fields in a structure of minimal energy.

The translation bound for the energy corresponds to the 3×3 matrix block $\hat{D}_i = k_i I_3$ and the projected translator $\hat{T}$ as in (18) where $|t| \le k_1$. Let the vector $\hat{E}_0$ be composed of the magnitudes of three loadings $\hat{E}_0 = (e_1, e_2, e_3)$. (That is, $\hat{E}_0$ is the projection of the diagonal components of the external fields E_0.) The most restrictive bound corresponds to $t = -k_1$. Then $\hat{D}_1 - \hat{T}$ becomes a diad

$$\hat{D}_1 - \hat{T} = 3k_1 l\, l^T, \quad l = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

The remaining matrices $\hat{D}_m - \hat{T}$ for $m = 2, ..., N$ are positive definite and have the representation

$$\hat{D}_k - \hat{T} = (k_m + 2k_1) l\, l^T + (k_m - k_1)(I - l\, l^T).$$

The projection of the field in the first phase of a translation-optimal structure is computed according to the case 2 as

$$\hat{E}_1 = \frac{k_* + 2k_1}{3k_1} l^T \hat{E}_0 l + (I - ll^T)\omega$$

where ω is a vector function in Ω_1 satisfying

$$\int_{\Omega_1} (I - ll^T)\omega \, dx = (I - ll^T)\hat{E}_0.$$

Notice that $\hat{E}_1$ is not completely defined: the vector function ω is free to vary in Ω_1. Since h is always orthogonal to l, this variation does not effect translated energy of the structure. The projected fields in the other phases fall into the case 1:

$$\hat{E}_m = \frac{k_* + 2k_1}{k_m + 2k_1} l^T \hat{E}_0 l, \quad m = 2, ..., N.$$

In particular, in the three-material case ($N = 3$) with diagonal fields discussed in the next section, we can summarize these properties as follows.

(P1) $\mathrm{Tr}(\nabla u(x)) = 3\tau_1$ in Ω_1,
(P2) $\nabla u(x) = \tau_2 I_3$ in Ω_2,
(P3) $\nabla u(x) = \tau_3 I_3$ in Ω_3,

where

$$\tau_i = \frac{k_* + 2k_1}{k_i + 2k_1}(l^T \hat{E}_0) \quad \text{for } i = 1, 2, 3.$$

Summing up the energy of these fields, we can also derive the standard formula (which coincides with the results of Hashin and Shtrikman Hashin and Shtrikman (1962) in this isotropic case) for the effective conductivity $K_* = k_* I$ of an isotropic translation-optimal N-material composite:

$$\frac{1}{k_* + 2k_1} = \sum_{i=1}^{N} \frac{m_i}{k_i + 2k_1}.$$

3. The modified differential scheme

In this section, we describe a convenient method for finding optimal multimaterial structures, using a modification of the the so-called *differential scheme*. The traditional differential scheme uses the strategy of inserting infinitesimal inclusions into an existing composite and calculating the increment of its effective properties. It is an old idea. Bruggeman used it in the thirties Bruggemann (1935) to compute effective properties. Later, the scheme was reinvented in the papers Norris (1985); Lurie and Cherkaev (1985), and was used for computing effective conductivity of an optimal polycrystal in Avellaneda et al. (1988). Generalizations of the scheme were suggested in Hashin (1988). The scheme we have chosen produces a rather general class of infinite-rank laminates. Keeping the previous section in mind, we also modify the traditional scheme to incorporate the optimality conditions of the fields at each step.

The particular variant of the scheme we use allows us to assemble an isotropic composite from anisotropic materials (or material mixtures). At every step in the process the composite we have constructed is isotropic. The process is equivalent to the following process which may be more easy to visualize. Starting with an infinitesimal spherical "seed" of some material, We repeatedly wrap an infinitesimal spherical shell of a transversal isotropic material around the current core, to grow a slightly larger core. The material in the shell is oriented so that the eigenvector for the differing eigenvalue points toward the center of the sphere.

In the following discussion, we apply this scheme to two examples. In the case of three-dimensional polycrystals, the solution was found in Avellaneda et al. (1988). Using the modified differential scheme, we observe that the fields indeed satisfy the optimality conditions (20) at every step of the process.

The second case is that of three-dimensional composites made from three isotropic conducting materials. In this case, the differential scheme contains a control which is free to vary at each infinitesimal step of the process. Rather than apply classical control theory to this problem, we show that if the volume fractions of the three materials lie in a certain range, we can obtain the optimal control by ensuring that the conditions (P1)-(P3) hold at every step of the process.

Strategy. We first describe an isotropic differential scheme that can produce optimal structures for both the problem of polycrystals and of three-component mixtures. The structure is obtained by a symmetric procedure which maintains isotropy at each step. An infinitesimal step is as follows. Three orthogonal infinitesimal strips with thickness $\frac{1}{3}\delta\mu$ in the current periodicity cell (which has conductivity $K_{\text{core}}(\mu) = k_{\text{core}}(\mu)I$) are replaced by a transversal isotropic composite with the conductivity tensor

$$K_{add} = \text{Diag}(k_n, k_t, k_t)$$

and its rotated triplets. Each strip is oriented so that the two eigenvectors for the eigenvalue k_t are parallel to the interface of the lamination while the third eigenvector is oriented along the normal. After each infinitesimal addition, the new composite is homogenized to find the new value of the conductivity $K_{\text{core}}(\mu + \delta\mu)$. Figure 1 illustrates the replacement of the orthogonal strips in one infinitesimal step.

Assume that the field in the core is proportional to identity

$$E(\mu) = \beta(\mu)I_3 = \beta(\mu)\text{Diag}(1, 1, 1)$$

The jump conditions require that the tangential components of the fields and the normal components of the currents are continuous across interfaces. The field in the added material is in rank-one connection with the core. In

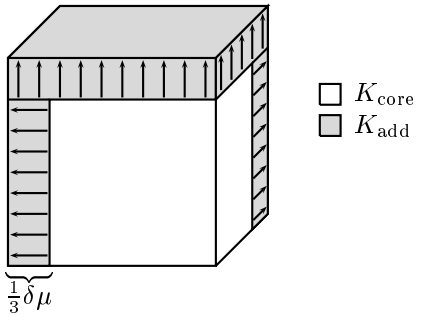

FIGURE 1. Replacing orthogonal strips in the differential scheme. The arrows in the added material indicate the direction of the conductivity eigenvalue k_n.

particular, the fields in the added layers must be (up to terms of order $\delta\mu$)

$$E_{x1} = \beta(\mu)\text{Diag}(\alpha(\mu), 1, 1), \quad n_{x1} = (1, 0, 0) \tag{21}$$

$$E_{x2} = \beta(\mu)\text{Diag}(1, \alpha(\mu), 1), \quad n_{x2} = (0, 1, 0) \tag{22}$$

$$E_{x3} = \beta(\mu)\text{Diag}(1, 1, \alpha(\mu)), \quad n_{x3} = (0, 0, 1) \tag{23}$$

where $\alpha(\mu) = \frac{k_{\text{core}}(\mu)}{k_n(\mu)}$. Thus, the field in the core, βI changes like

$$\beta(\mu + \delta\mu) = \left(1 - \frac{1}{3}\delta\mu\right)\beta(\mu) + \frac{1}{3}\delta\mu(\beta(\mu)\alpha(\mu) + O(\delta\mu)). \tag{24}$$

Letting $\delta\mu \to 0$, we find

$$\beta' = \frac{1}{3}\beta(\alpha - 1) \tag{25}$$

We can also track the relative volume fraction m_{core} of the core in the evolving structure and its effective properties $k_{\text{core}}(\mu)$. Because of relation

$$m_{\text{core}}(\mu + \delta\mu) = (1 - \delta\mu)m_{\text{core}}(\mu), \tag{26}$$

we find

$$m'_{\text{core}} = -m_{\text{core}}, \quad \text{and} \quad m_{\text{core}}(0) = 1 \tag{27}$$

and therefore

$$m_{\text{core}}(\mu) = e^{-\mu}. \tag{28}$$

The effective conductivity evolves as follows Cherkaev (2000).

$$k'_{\text{core}}(\mu) = k_{\text{core}}(\mu)\frac{k_n(\mu) - k_{\text{core}}(\mu)}{3k_n(\mu)} + \frac{2}{3}(k_t(\mu) - k_{\text{core}}(\mu)). \tag{29}$$

We add two modification to the conventional scheme to adjust it to the optimization problem.

(1) We allow the addition of not only pure materials, but also composite materials, such as laminates.

(2) We track the fields in each material at each step. Because we know the field in the added composite, we know the fields in each component. We use this information to choose the composite to ensure that the optimality conditions are satisfied at every point.

3.1. **Polycrystal and non-rank-one-connected fields.** The translation-optimal fields (20) are not rank-one connected. Therefore, there is no finite-rank laminate that can attain the translation bound. However, the bound is attainable by the infinite-rank structure as is demonstrated in Avellaneda et al. (1988). Here, we comment on the fields in the optimal structure. In order to initiate the differential scheme, we add an isotropic material K_{isotr} into the polycrystal, choosing it so that the field in it,$E_0 = \beta_0, I$ is rank-one connected to an optimal field in each of the anisotropic phases. In particular, we can take $\tau = \beta_0$ in each of the cases of (20). We then modify the core by the differential scheme described above.

To simplify the calculations, we choose to keep K_{core} constant. To do this, we choose the conductivity of the core $K_{\text{isotr}} = k_{\text{isotr}} I$ so that the right-hand side of (29) vanishes. (We set $k_t \equiv 1$ and $k_n \equiv s$.) We then compute

$$k_{\text{isotr}} = k_{\text{core}}(\mu_0) = k_0 = \frac{1}{2}\left(\sqrt{s^2+8s} - s\right).$$

Then $k_{\text{core}}(\mu) = k_0$ stays constant for all μ, but the volume fraction of the isotropic seed K_{isotr} used in the composite goes to zero as $\mu \to \infty$.

Notice that the field $E(\mu) = \beta(\mu) I$ stays isotropic, therefore the fields in the added infinitesimal layers have the form

$$\beta(\mu)(I + n\, n^T(\alpha - 1)),$$

and $\alpha = \frac{k_0}{k_n} = \gamma_1$ is constant. Comparing this with (20) we observe that the fields are translation-optimal pointwise.

Then, from (25) we compute the value, β, of the magnitude of the fields in the added crystallites,

$$\beta(\mu) = \beta_0 e^{(\alpha-1)\mu/3} \tag{30}$$

where β_0 is the value of β in the core: $\beta_0 = \beta(0)$.

We see from (27) that as $\mu \to \infty$ the volume fraction of the core vanishes. Thus, in the limit we obtain a composite with pointwise-optimal (and incompatible!) fields.

Remark. Notice that the case described is similar to the example of the quasiconvex envelope supported by four incompatible fields, which is discussed in several papers such as Pedregal (1993); Tartar (1993); Nesi and Milton (1991). The similarity lies in the fact that an infinite rank laminate is necessary to join the fields; no finite rank laminate is sufficient. The present problem is slightly more complex, using infinitely many fields along the three lines. On the other hand, while the four-field problem is quite artificial, the present three-dimensional problem originates from a problem with a clear physical meaning.

3.2. **Optimal three-material structures.** The differential scheme also allows us to find isotropic translation-optimal structures for multimaterial mixtures. We use it here to find new translation-optimal structures for three-material composites. A class of such structures (the so-called "coated spheres") was introduced in the papers Milton (1981); Milton and Kohn (1988). According to this construction the amount of k_1 is split into two parts. Each part is used together with k_2 and k_3, respectively, to form two-material *coated spheres* so that k_1 is the envelope and the other material is the core. If the effective properties of the coated spheres are equal to each other, they can be mixed together forming an optimal multimaterial isotropic composite. The fields in the cores are isotropic and one can check that all the fields satisfy the sufficient conditions (P1)-(P3). This construction is geometrically possible if and only if the volume fractions of the materials satisfy the applicability condition

$$\eta \le m_1 \le 1, \quad \eta := \frac{3k_1(k_3-k_2)}{(k_2+2k_1)(k_3-k_1)}(1-m_2). \tag{31}$$

In the following discussion, we introduce another type of optimal structure ("hairy spheres", perhaps) that are geometrically possible for a larger range of m_1:

$$\eta^* \le m_1 \le 1, \quad \eta^* := \frac{3k_1(k_3-k_2)}{(k_2+2k_1)(k_3-k_1)}(\sqrt[3]{m_2}-m_2). \tag{32}$$

Note that

$$\frac{\eta^*}{\eta} = \frac{\sqrt[3]{m_2}-m_2}{1-m_2} \le \frac{2}{3} \quad \text{and} \quad \lim_{m_2\to 0}\frac{\eta^*}{\eta} = 0.$$

Thus, for fixed m_2, the structures we introduce are always possible for a larger range of m_1 than the coated spheres structures. As $m_2 \to 0$, this difference becomes pronounced.

The structures. Consider a three-material translation-optimal composite. The fields in the phases are described by (P1)-(P3). The following construction generates optimal isotropic microstructures. We begin with an initial core of the second material k_2. Then at each step in the differential scheme process, we can chose to add either

(1) three orthogonal layers of a transversal-isotropic composite K_{13} of materials k_1 and k_3 formed by placing a cylindrical inclusion of k_3 into a matrix of k_1, or
(2) three orthogonal layers of pure material k_1.

Any of these additions keeps the field translation-optimal.

The infinitesimal layers of K_{13} are always oriented so that the axis of cylindrical inclusions in K_{13} coincides with normal to the layer. The volume fraction $\nu(\mu)$ of the matrix (or $1-\nu(\mu)$ of the cylindrical inclusions) is chosen so that the fields satisfy the optimality conditions at every step as we discuss below. Because of this requirement, we find that $\nu(\mu)$ decreases with μ.

The infinitesimal layers of pure k_1 have no volume fraction control. They can always be added because of the freedom provided the field in k_1 by (P1). Indeed, if the core has isotropic fields βI, then the field $\mathrm{Diag}(\beta, \beta, 3\tau_1 - 2\beta)$ and its two permutations satisfy (P1) and are in rank-one connection with the core.

We can continue this process as long as we like alternating between the two types of inclusions. This procedure can produce optimal composites for fixed volume fraction provided the volume fractions of components are subject to some constraints.

Remark. While it is impossible to describe the infinite-rank laminate in finite length scales, the following coated spheres structure is useful for visualizing its main features. A spherical core of k_2 is surrounded by a spherical layer of k_1 stuffed with radially-oriented conical inclusions (hairs) of k_3. The cones become thicker with the increase of the radius to some point and then stop. Then, this sphere is optionally enveloped by the remaining portion of k_1 that forms an outer spherical shell.

Fields in the added composites with cylindrical inclusions. The three-dimensional transversally isotropic extremal structure with cylindrical inclusions can be assembled either as coated cylinders, or as second-rank matrix laminates, or as Vigdergauz-type structures Cherkaev (2000); Milton (2002). In all these constructions, one can check that if the field in the cylindrical inclusion is the isotropic constant field $\tau_3 I$, then the average field in the composite is given by

$$\frac{1}{2}\tau_3 \mathrm{Diag}\left(2, \nu\frac{k_3}{k_1} + (2-\nu), \nu\frac{k_3}{k_1} + (2-\nu)\right)$$

if the normal is $(1,0,0)$ and a properly rotated matrix for the other two normals. Here ν is the relative volume fraction of k_1 in the composite. In particular, to bring this field into rank-one connection with the core, we need to choose

$$\nu = \frac{2k_1(\beta - \tau_3)}{\tau_3(k_3 - k_1)}.$$

Of course, this is only possible if $0 \le \nu \le 1$ or

$$\frac{k_3 + k_1}{2k_1}\tau_3 \le \beta \le \tau_3.$$

It is easy to check that this constraint is satisfied for every step of the differential scheme if $\beta(0) = \tau_2$: the optimal field in material k_2.

The evolution of the field in the core is described by (25); this time both β and α depend on μ. The varying fraction ν in the added laminate is chosen to keep the fields in the structure optimal. By solving for α and then β, we can find the fraction ν depending on μ; it decreases with μ as follows.

$$\nu(\mu) = \frac{2k_1(k_3 - k_2)}{(k_2 + 2k_1)(k_3 - k_1)}\, e^{-\mu/3}.$$

Comparison to previous structures. In order to compare these structures to the previously known optimal structures, we need to compute the relative volume fractions in the final composite. If no layer of pure k_1 is added (only "hairs") then the construction uses the minimal amount of k_1. In this case, the volume fractions in the differential scheme satisfy the ordinary differential equations

$$m_1'(\mu) = \nu(\mu) - m_1(\mu), \quad m_1(0) = 0$$

and

$$m_2'(\mu) = -m_2(\mu), \quad m_2(0) = 1.$$

Solving, we find

$$m_2(\mu) = e^{-\mu}, \quad m_1(\mu) = \frac{3k_1(k_3 - k_2)}{(k_2 + 2k_1)(k_3 - k_1)} \left(e^{-\mu/3} - e^{-\mu} \right).$$

In particular, we find the volume fractions of the final composite by substituting:

$$m_1 = \eta^* = \frac{3k_1(k_3 - k_2)}{(k_2 + 2k_1)(k_3 - k_1)} \left(\sqrt[3]{m_2} - m_2 \right)$$

Observe that this value of m_1 is below the bound of applicability (31) of the coated spheres construction. Additionally, since we can coat this structure with layers of k_1, we find the condition for applicability of the modified differential scheme is (32). In this sense, the differential scheme generalizes and improves upon previous results. It requires less amount of k_1 than the coated spheres.

Remark. The following is a useful visualization for explaining why the new structures can mimic the coated spheres. We imagine beginning with the core of K_2 and applying rule 1 above to form a thin layer of the cylindrical inclusions. This generates a new structure whose effective conductivity lies a bit above K_2. Now apply rule 2 to add a thin layer of pure K_1. We add just enough to bring the effective tensor back to K_2. We can continue to repeat this two-step procedure as often as we want, decreasing m_2 and increasing m_1 and m_3 as long as we wish, always bringing the effective conductivity back to K_2 each time. Visualized in this way, the cylindrical inclusions of K_3 are "cut short" and resemble spheres surrounded in a matrix of K_1. It is also interesting to visualize the new structures in this way. We simply elongate the spheres of K_3 in the radial direction until they join and form "hairs".

This construction is easily extended to larger numbers of materials ($N > 3$). Choosing the initial core to be k_2 was convenient, but we may start with any core we wish. At any step, we may add one of up to N different types of layers: $N - 1$ types of a cylindrical inclusion in k_1 or a layer of pure k_1. Some bookkeeping is required, but the idea is straightforward. At any step we can add either pure k_1 or any coated cylinder composite for which we can choose the volume fractions to satisfy (P1)-(P3). We also note that the

assembly of coated spheres also extends to many materials. In all cases, the applicability conditions for the coated spheres are stricter than those of the structures described in this paper.

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