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Rank-three laminates are good approximants of the optimal microstructures for the diffusion problem in dimension two

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Abstract

In two dimensions there are optimal bounds for the effective conductivity of arbitrary mixtures of two heat conducting materials: one isotropic and the other anisotropic; used in fixed volume fractions and allowing for rotations. Some of those bounds involve a rank-two lamination, but others involve a microstructure of coated disks. We create a region of laminates of rank at most three, which gives a very good approximation of the optimal bound if the starting material has a moderate degree of anisotropy. We also study the stability under homogenization of this region, meaning that whenever one homogenizes a mixture of two materials belonging to it, the effective diffusion tensor also belongs to this region. This is done to show that the region we create cannot be easily enlarged.

Keywords: Composites; Homogenization; Laminates

1. Introduction

The role of the microstructure in determining the macroscopic, or effective, behavior of a composite material is by now a well-known feature. Some important advances have been obtained lately in getting a full solution to the problem of characterizing the set $\mathscr{G}_\theta$ of the diffusion tensors that can be constructed through arbitrary mixtures of two heat conducting materials or phases: one isotropic and the other anisotropic; when they are used in fixed volume fractions: θ for one of them and $1-\theta$ for the other, and allowing for rotations.

Once an optimal bound has been found, if the microstructure that saturates the bound is not simple, it arises the question of how far from optimal are simple microgeometries, like low-rank laminates. This is the problem studied here in three aspects: creating a particular set of laminates of rank at most three that will be close to $\mathscr{G}_\theta$, studying the stability of such set under homogenization and finally quantifying the difference between that set and $\mathscr{G}_\theta$, or a good candidate for it.

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The Theory of Homogenization deals with computing the macroscopic behavior of a material that is inhomogeneous at a much smaller scale. This scale, however, cannot be too small since the phenomenon is always described by the equations of continuous media. On its deterministic variant it considers a fixed microstructure, for example a periodic array, and it tries to determine whether the behavior of the material becomes in average similar to that of a homogeneous material at scales larger and larger. The subtle point is to give a precise meaning to this average behavior: for a problem of steady-state heat conduction one requires that the temperature fields and also the heat fluxes become closer and closer to those of the homogeneous material; for elastostatics one requires that the deformation and the strain and stress tensors become progressively closer to those of the homogeneous material. But now the question is to make precise the meaning of this closeness. Since we want the macroscopic behavior of the samples of material to be very similar, we consider macroscopic measurements of the quantities we require to be similar. However a macroscopic measurement necessarily involves taking some kind of average at a smaller length scale and this averaging technique has to be sufficiently robust because we will be averaging quantities that tend to vary very fast, since we will use larger and larger length scales. The answer to this crucial point is the notion of weak convergence, which came mostly in the past century, from the work of many scientists: mathematicians, physicists and engineers.

Let us now be more precise and recall the mathematical definition of H-convergence of Murat and Tartar, in the context of steady-state diffusion of heat, see for example Murat and Tartar (1983), and which is based on weak convergence. Even though we do not use it explicitly in the following work, it will always be on the background. It is similar to G-convergence, introduced by Spagnolo with a different purpose, except that H-convergence does not require the tensors involved to be symmetric, which is of no consequence here, since diffusion tensors are always symmetric. Let Ω be a regular open subset of $\mathbb{R}^2$ and $\{\mathbf{A}^n\}$ be a sequence of diffusion tensors. Then we say that $\mathbf{A}^n$ H-converges to $\mathbf{A}^{\text{eff}}$ if for all $f \in H^{-1}(\Omega)$ we have a subsequence of $\{u^n\} \subset H_0^1(\Omega)$, solutions to

$$\left.\begin{array}{l} -\operatorname{div}(\mathbf{A}^n \operatorname{grad} u^n) = f \quad \text{in } \Omega \\ u^n = 0 \quad \text{on } \partial\Omega, \end{array}\right\}$$

which satisfies that $u^n \to u^\infty$ weakly in $H_0^1(\Omega)$ and $\mathbf{A}^n \operatorname{grad} u^n \to \mathbf{A}^{\text{eff}} \operatorname{grad} u^\infty$ weakly in $L^2(\Omega, \mathbb{R}^2)$, where u^∞ is the solution to

$$\left.\begin{array}{l} -\operatorname{div}(\mathbf{A}^{\text{eff}} \operatorname{grad} u^\infty) = f \quad \text{in } \Omega \\ u^\infty = 0 \quad \text{on } \partial\Omega. \end{array}\right\}$$

The meaning of this somewhat involved definition is that for any heat source f, the behavior of the $\mathbf{A}^n$s becomes more and more similar to that of $\mathbf{A}^{\text{eff}}$ in terms of the weak limits of both: the induced temperature field u^n and the induced heat flux $\mathbf{A}^n \operatorname{grad} u^n$. In the context of finding $\mathscr{G}_\theta$, the $\mathbf{A}^n$s are discontinuous diffusion tensor-fields that take only two values, namely those corresponding to the two materials we are mixing, and for each microstructure we have a different way in which $\mathbf{A}^n$ varies in space.

The problem of finding $\mathscr{G}_\theta$ is sometimes referred to as the G_θ-closure problem, as a variation of the G-closure problem. The question of characterizing $\mathscr{G}_\theta$, or variations of it, has been extensively studied in the last three decades. Some of the classical references are: Tartar (1977, 1985), Murat and Tartar (1983), Cherkaev and Lurie (1984a), Francfort and Murat (1987) and Milton and Nesi (1999). For a recent account on the state of the art in this subject (see Allaire, 2002). The situation when both starting materials are isotropic was completely solved in Murat and Tartar (1983), Tartar (1985), Cherkaev and Lurie (1984a,b). If one of the starting materials is allowed to be anisotropic, in Nesi (1993) an optimal bound was obtained for anisotropic composites on the side of the region closer to the isotropic phase, but to show the attainability of the bound a constraint on θ has to be imposed. Later in Nesi (1996) an optimal bound was proved on the other side of the region, but only for isotropic composites. Finally on case II as defined below, in Milton and Nesi (1999) the full characterization of $\mathscr{G}_\theta$ was obtained, still under the same constraint on θ mentioned before. For case I there is only a corresponding conjecture coming from Astala and Miettinen (1998). We recall these results in Section 2.

We will have mixtures of two phases: material a with diffusion tensor $\mathbf{A}$ is used in volume fraction θ, $\theta \in (0,1)$; the other is material b with diffusion tensor $\mathbf{B}$. We divide the study in two cases:

Case I. $\mathbf{A} = \alpha I$, $\mathbf{B} = \mathrm{diag}(\beta, \gamma)$ and $\alpha^2 < \beta\gamma$.
Case II. $\mathbf{A} = \mathrm{diag}(\alpha, \beta)$, $\mathbf{B} = \gamma I$ and $\alpha\beta < \gamma^2$.

In Section 3 we make the explicit construction of a region of laminates of rank at most three, denoted by $\mathscr{L}_\theta$, and show at least in some cases that this region is H-stable, meaning that whenever we homogenize a mixture of two materials belonging to this region, the resulting effective tensor also belongs to the same region. This means that despite the simplicity of the microstructures used to generate the tensors in $\mathscr{L}_\theta$, they can reproduce almost all the possible effective tensors, as it will be numerically shown in the last section, and it also means that to get an even better approximation, most likely one needs to use a complicated microgeometry. First in Section 3.1 we recall a result from Francfort and Murat (1987), quoted below as Theorem 3.1, which gives sufficient conditions for a set of tensors to be H-stable. This theorem requires two main hypothesis, on the one hand that the boundary be C^1, this is that the boundary is formed by functions that are differentiable with the derivative being continuous, and on the other hand that the region be enclosed between a convex and a concave function. We then extend that result to get Proposition 3.4 by relaxing the former hypothesis to cover the case of the explicit construction we present in Section 3.2, this is of a curve of rank-two laminates almost enclosing a region whose interior and a small piece of its boundary are obtained by one more lamination. Then in case I and if we further restrict ourselves to the well-ordered case (see Francfort and Murat, 1987), i.e. we also require that α be less than both β and γ, we can prove using Proposition 3.4 that $\mathscr{L}_\theta$ is H-stable. For the non-well-ordered case we could not do such general verification, instead we checked numerically that the second derivatives of the bounding functions do have the right signs, to do it we discretize the values taken by θ over the whole interval $(0,1)$, fix $\alpha = 1$ and $\gamma = 5$ and discretize β over the interval $(0.2, 5)$. We present the analogous construction for case II in Section 3.3 and again checked numerically the sign of the derivatives, the only difference being that now β will be discretized over the interval $(1, 25)$. Therefore there is very strong evidence that $\mathscr{L}_\theta$ is always H-stable.

Finally in Section 4 and for the same discretizations mentioned above, we compute the difference between the optimal bound and the conductivity of the closest isotropic conductor belonging to $\mathscr{L}_\theta$, on the side of the region closer to the anisotropic phase. Restricting the ratio between the conductivities of the anisotropic phase to be at most 25, we obtain that rank-three laminates will yield a composite with an effective conductivity very close to the optimal value, the maximum difference being of about 2%, gain which most probably will be offset by the cost of having to use a much more complicated assembling procedure. On the other side of the region there is no gap if the volume constraint imposed by either Theorem 2.1 or 2.2 is met.

Throughout the paper we denote by e_i the ith canonical vector and say that the lamination is in the direction of $\zeta \in \mathbb{R}^2$, $\zeta \neq 0$, if the interfaces between the laminates are perpendicular to ζ.

2. Optimal bounds

Here we recall the known optimal bounds and one conjecture for it. First we present the results using quasiconformal mappings obtained in Astala and Miettinen (1998) and Milton and Nesi (1999), which to show the attainability of the bounds, uses a microstructure following the construction of Hashin-Shtrikman and Schulgasser, since it involves constructing disks of different sizes that always have one eigenvector of the anisotropic phase pointing towards the center of the disk. The other optimal bound, to be recalled secondly, comes from a simple rank-two laminate and was obtained in Nesi (1993).

Following Nesi (1993) let us define the following quantities, which give the values of the two conductivities of a rank-one laminate between the phases in the prescribed volume fractions for each of the cases. In case I if the laminate is in the e_1 direction

$$h_1^{\mathrm{I}}(\theta) = \left(\frac{\theta}{\alpha} + \frac{1-\theta}{\beta}\right)^{-1} \quad \text{and} \quad a_2^{\mathrm{I}}(\theta) = \theta\alpha + (1-\theta)\gamma,$$

and if the laminate is in the e_2 direction

$$h_2^{\mathrm{I}}(\theta) = \left(\frac{\theta}{\alpha} + \frac{1-\theta}{\gamma}\right)^{-1} \quad \text{and} \quad a_1^{\mathrm{I}}(\theta) = \theta\alpha + (1-\theta)\beta.$$

In case II if the laminate is in the e_1 direction

$$h_1^{\mathrm{II}}(\theta) = \left(\frac{\theta}{\alpha} + \frac{1-\theta}{\gamma}\right)^{-1} \quad \text{and} \quad a_2^{\mathrm{II}}(\theta) = \theta\beta + (1-\theta)\gamma,$$

and for the e_2 direction

$$h_2^{\mathrm{II}}(\theta) = \left(\frac{\theta}{\beta} + \frac{1-\theta}{\gamma}\right)^{-1} \quad \text{and} \quad a_1^{\mathrm{II}}(\theta) = \theta\alpha + (1-\theta)\gamma.$$

In case I $\mathscr{G}_\theta$ is not known, instead we have a region $\widetilde{\mathscr{G}}_\theta$ enclosed by two curves, one presented in (2.2) is only conjectured to be a bound while the other, coming from (2.3), is a bound which is fully attained provided that $a_1^{\mathrm{I}} \geqslant h_2^{\mathrm{I}}$, which imposes a lower bound for θ.

In case II $\mathscr{G}_\theta$ is enclosed by two curves, one presented in (2.1) and the other coming from (2.4), which is fully attained under the assumption that $a_1^{\mathrm{II}} \geqslant h_2^{\mathrm{II}}$, which now translates into an upper bound for θ.

2.1. Using quasiconformal mappings

Nesi (1996) introduced the idea of using quasiconformal mappings and obtained optimal bounds, either from above or from below, depending on the case, but only for isotropic composites belonging to $\mathscr{G}_\theta$. Case I is covered by Theorem 5.3 in Nesi (1996), while case II is covered by Theorem 5.2 in that paper. Then in Astala and Miettinen (1998), the authors conjectured optimal bounds working on the side of $\mathscr{G}_\theta$ closer to the anisotropic phase, one for each of the situations studied by Nesi. Lately in Milton and Nesi (1999) the conjecture of Astala and Miettinen covering case II was proved, which we now recall. From (4.1) and (4.2) in Milton and Nesi (1999) written in our notation, let be:

$$d_1 = \sqrt{\alpha\beta}, \qquad K = \sqrt{\frac{\beta}{\alpha}}, \qquad A = \frac{d_1 - \gamma}{d_1 + \gamma}$$

and

$$S(t) = -d_1 + \frac{2d_1}{1 + At^K} \quad \forall t \in [0, 1],$$

where t represents the volume fraction of material b. The material with diffusion tensor $S(t)I$ is obtained by filling the domain with disks of varying sizes and which are constructed following the Hashin-Shtrikman–Schulgasser idea, namely with a core of the isotropic phase and an annulus of the anisotropic phase with the less conducting direction always pointing to the center of the disk. $S(1-\theta)$ gives an optimal lower bound for the conductivity of the isotropic materials belonging to $\mathscr{G}_\theta$ (see Theorem 4.2 in Milton and Nesi, 1999).

Then using an isotropic material constructed in this way and relaminating it with the anisotropic phase, in the direction of e_1, they got (see Proposition 5.2 in Milton and Nesi, 1999) an optimal lower bound given by the curve of materials with conductivities

$$\lambda_1 = \left(\frac{\xi_1}{S(\xi_2)} + \frac{1-\xi_1}{\alpha}\right)^{-1} \quad \text{and} \quad \lambda_2 = \xi_1 S(\xi_2) + (1-\xi_1)\beta, \tag{2.1}$$

where $\xi_1, \xi_2 \in [0,1]$ and $\xi_1\xi_2 = 1-\theta$.

The other conjecture of Astala and Miettinen has not been proved, to the best of our knowledge. The curve coming from this conjecture together with the curve coming from the optimal bound proved in Theorem 2.1, enclosed a region that we denote by $\widetilde{\mathscr{G}}_\theta$. From formula (5.4) in Astala and Miettinen (1998), written in our notation, we set:

$$\delta = \sqrt{\beta\gamma}, \qquad K = \sqrt{\frac{\gamma}{\beta}} \qquad A = \frac{\delta(\alpha-\delta)}{\alpha+\delta}$$

and

$$S(t) = \left(\frac{2}{\delta + At^K} - \frac{1}{\delta}\right)^{-1} \quad \forall t \in [0,1],$$

where t represents now the volume fraction of material a. Then, repeating the process as before, one gets a curve of materials with conductivities

$$\lambda_1 = \left(\frac{\xi_1}{S(\xi_2)} + \frac{1-\xi_1}{\beta}\right)^{-1} \quad \text{and} \quad \lambda_2 = \xi_1 S(\xi_2) + (1-\xi_1)\gamma, \tag{2.2}$$

where $\xi_1, \xi_2 \in [0,1]$ and $\xi_1\xi_2 = \theta$, which would give the optimal upper bound.

2.2. Optimal rank-two laminates

In Nesi (1993), among many other results, two optimal bounds were proved concerning the G_θ-closure of any pair of materials, one isotropic and the other anisotropic, in any dimension greater than or equal to two (see Section 7.3 in Nesi, 1993).

Theorem 2.1. *Let $\alpha, \beta, \gamma \in \mathbb{R}^+$ be such that $\alpha^2 < \beta\gamma$ and $\theta \in (0,1)$. Let then be material a with diffusion tensor $A = \alpha I$ and material b with diffusion tensor $B = \operatorname{diag}(\beta,\gamma)$. Then if λ_1 and λ_2 are the main conductivities of a homogeneous material created by mixing material a in proportion θ and material b or rotations of it in proportion $1-\theta$, we have that*

$$\frac{\alpha}{\lambda_1-\alpha} + \frac{\alpha}{\lambda_2-\alpha} \leqslant \frac{S_1}{1-S_1} = \frac{1}{1-\theta}\left(\theta + \frac{\alpha}{\beta-\alpha} + \frac{\alpha}{\gamma-\alpha}\right), \tag{2.3}$$

where

$$S_1 = \theta + (1-\theta)\frac{\alpha(\beta+\gamma) - 2\alpha^2}{\beta\gamma - \alpha^2}.$$

Furthermore the bound (2.3) is attained by rank-two laminates and under the assumption that $a_1^{\mathrm{I}} \geqslant h_2^{\mathrm{I}}$, which means that $\theta \in [\theta^{\mathrm{I}}_{\min}, 1)$, where

$$\theta^{\mathrm{I}}_{\min} = \frac{\alpha(\gamma-\beta)}{(\beta-\alpha)(\gamma-\alpha)},$$

the whole curve in the box $[h_1^{\mathrm{I}}, a_2^{\mathrm{I}}] \times [h_1^{\mathrm{I}}, a_2^{\mathrm{I}}]$ *on the* (λ_1, λ_2)*-plane given by equality in* (2.3) *is realized by rank-two laminates.*

Theorem 2.2. *Let* $\alpha, \beta, \gamma \in \mathbb{R}^+$ *be such that* $\alpha\beta < \gamma^2$ *and* $\theta \in (0, 1)$. *Let then be material a with diffusion tensor* $A = \mathrm{diag}(\alpha, \beta)$ *and material b with diffusion tensor* $B = \gamma I$. *Then if* λ_1 *and* λ_2 *are the main conductivities of a homogeneous material created by mixing material a or rotations of it in proportion* θ *and material b in proportion* $1 - \theta$, *we have that*

$$\frac{\lambda_1}{\gamma - \lambda_1} + \frac{\lambda_2}{\gamma - \lambda_2} \leqslant \frac{S_2}{1 - S_2} = -1 + \frac{1}{\theta}\left(1 + \frac{\alpha}{\gamma - \alpha} + \frac{\beta}{\gamma - \beta}\right), \tag{2.4}$$

where now

$$S_2 = \theta \frac{\gamma(\alpha + \beta) - 2\alpha\beta}{\gamma^2 - \alpha\beta} + 1 - \theta.$$

Furthermore the bound (2.4) *is attained by rank-two laminates and under the assumption that* $a_1^{\mathrm{II}} \geqslant h_2^{\mathrm{II}}$, *which means that* $\theta \in (0, \theta_{\max}^{\mathrm{II}}]$, *where*

$$\theta_{\max}^{\mathrm{II}} = 1 - \frac{\gamma(\beta - \alpha)}{(\gamma - \alpha)(\gamma - \beta)},$$

the whole curve in the box $[h_1^{\mathrm{II}}, a_2^{\mathrm{II}}] \times [h_1^{\mathrm{II}}, a_2^{\mathrm{II}}]$ *on the* (λ_1, λ_2)*-plane given by equality in* (2.4) *is realized by rank-two laminates.*

In both cases the optimal microstructure is produced through an iterated lamination with the isotropic phase, first one laminates the anisotropic material with the isotropic phase in the direction of e_1 and then laminates the outcome of this with the isotropic phase, but now in the direction of e_2. We have recently found and alternative proof of these bounds, using only the Homogenization method as presented in Tartar (2000) (see Gutiérrez, in press).

3. *H*-stability

As we said in the Introduction, in Francfort and Murat (1987) was defined the concept of H-stability. In that article this idea was used to fully characterize the set of all possible mixtures of two anisotropic materials, but without fixing the proportions. We would like to use this idea to show that a region we can create by doing only laminates of rank at most three, is H-stable. We only succeeded in case I under the extra assumption that the tensors are well-ordered, which implies that $\alpha < \beta \leqslant \gamma$. For the other situations, we only verified the conditions numerically.

3.1. A characterization of H-stable regions

The following theorem was proved in Francfort and Murat (1987) and gives sufficient conditions to make a set of tensors to be H-stable. One of the conditions of the theorem is too strong and it will not be satisfied by our region, however it will not be hard to make the appropriate extension.

Theorem 3.1. *Let* δ_1 *and* δ_2 *be strictly positive real numbers such that*

$$\alpha_0^2 \leqslant \delta_1 \leqslant \delta_2 \leqslant \beta_0^2.$$

Let φ and ψ be two real-valued functions defined on $[\delta_1, \delta_2]$ with the following properties:

$$\begin{cases} \varphi \text{ and } \psi \text{ are } C^1 \text{ functions with values in } R_+^*, \\ \varphi \text{ is concave}, \\ \psi \text{ is convex}, \\ \varphi(d)\psi(d) = d \text{ for any } d \in [\delta_1, \delta_2]. \end{cases}$$

Define $K(\delta_1, \delta_2, \varphi, \psi)$ as the set of all $(\lambda_1, \lambda_2) \in [\alpha_0, \beta_0]^2$ such that $\delta_1 \leqslant \lambda_1\lambda_2 \leqslant \delta_2$ and $\psi(\lambda_1\lambda_2) \leqslant \lambda_1$, $\lambda_2 \leqslant \varphi(\lambda_1\lambda_2)$. Then the set of diffusion tensors that have their eigenvalues belonging to $K(\delta_1, \delta_2, \varphi, \psi)$, denoted by $\mathscr{M}(K(\delta_1, \delta_2, \varphi, \psi))$, is H-stable.

For the region K we construct, one part of its boundary comes from the optimal bound derived either in Theorem 2.1 or 2.2. The other part comes from an explicit rank-two lamination. The problem we run into is that the corresponding functions φ and ψ will not be differentiable at the point where both parts of the boundary meet, therefore we want to relax the C^1 requirement in Theorem 3.1, which is heavily used in its proof. To do it we use the following two lemmas:

Lemma 3.2. *The increasing union of sets which are H-stable is H-stable.*

Proof. If $\mathbf{A}_0$ and $\mathbf{B}_0$ belong to the union, then both belong to one of the sets in the union, so all the tensors produced by homogenizing mixtures using only those tensors also belong to that set and therefore to the union. □

Lemma 3.3. *Let $K \subset \mathbb{R}_+^2$ be a bounded set on the (d, λ)-plane, such that $\mathscr{M}(K)$ is H-stable, then if $\overline{K}$ denotes the closure of K, the set $\mathscr{M}(\overline{K})$ is also H-stable.*

Proof. If $\mathscr{M}(\overline{K})$ were not H-stable, there must exist $\mathbf{A}_0, \mathbf{B}_0 \in \mathscr{M}(\overline{K})$, whose representation on the (d, λ)-plane are, respectively, k and w, with $k, w \in \overline{K}$, and such that we can homogenize a mixture of them to get a tensor $\mathbf{C}_0 \notin \mathscr{M}(\overline{K})$. Then calling k^* the representation of $\mathbf{C}_0$ on (d, λ), we have that $k^* \notin \overline{K}$.

There are then two sequences of tensors in $\mathscr{M}(K)$ whose representations on the (d, λ)-plane, $\{k_m\}$ and $\{w_m\}$, belong to K and which converge in the norm of $\mathbb{R}^2$ to k and w, respectively. Let then $\{\mathbf{C}_n\}$ be the sequence of tensors mixing $\mathbf{A}_0$ and $\mathbf{B}_0$ and H-converging to $\mathbf{C}_0$. Now for each m, using the same micro-geometry and rotations of the tensors, we can construct another mixture using now tensors represented by k_m and w_m, to create a sequence of tensors $\{\mathbf{B}_n^m\}$, which due to sequential compactness of H-convergence, must have a subsequence which H-converges, let us say to $\mathbf{B}_0^m$ represented by k'_m.

Now, for any $\varepsilon > 0$ we can choose m large enough to make $|\mathbf{B}_n^m - \mathbf{C}_n| \leqslant \varepsilon$ pointwise and uniformly on n. But Proposition 16 of Tartar (2000) gives then that $|\mathbf{B}_0^m - \mathbf{C}_0|$ is bounded by a constant times ε, which in turn implies that the distance between k^* and k'_m should also be bounded by a constant times ε. Then by selecting ε sufficiently small, we conclude that $k'_m \notin K$, which contradicts the H-stability of $\mathscr{M}(K)$. □

Proposition 3.4. *Let K be as in Theorem* 3.1 *except that φ and ψ are continuous, but they may not be differentiable at a finite number of points in (δ_1, δ_2), where they have only directional derivatives and their one-sided derivatives at δ_1 and δ_2 might not be finite. Then we still have that $\mathscr{M}(K)$ is H-stable.*

Proof. The fourth condition on φ and ψ in Theorem 3.1 implies that the points where the functions are not smooth are common. Let then $T = \{d_i \in (\delta_1, \delta_2) : i = 1, \dots, m\}$ be that set of points, then for ε positive but sufficiently small, we construct a sequence of sets K_ε by doing two things: first we regularize φ and ψ on all the intervals $(d_i - \varepsilon, d_i + \varepsilon)$, so to make them C^1, and secondly, we also need to restrict $d \in [\delta_1 + \varepsilon, \delta_2 - \varepsilon]$, since both φ and ψ may not be differentiable at the end points. Then now the sets K_ε satisfy all the hypothesis of Theorem 3.1.

Hence, using Theorem 3.1, we have that all the sets $\mathscr{M}(K_\varepsilon)$ are H-stable, and $K_\varepsilon \subset K$, then applying Lemma 3.2 we get that

$$K' = K \setminus \left(\{(d_i, \varphi(d_i)), (d_i, \psi(d_i)) : i = 1, \ldots, m\} \cup \bigcup_{i=1}^{2} (\delta_i \times [\psi(\delta_i), \varphi(\delta_i)]) \right),$$

makes $\mathscr{M}(K')$ to be H-stable and then using Lemma 3.3, we conclude that K is such that $\mathscr{M}(K)$ is H-stable. □

3.2. Case I

We assume then that $\mathbf{A} = \alpha I$, $\mathbf{B} = \operatorname{diag}(\beta, \gamma)$ with $\alpha^2 < \beta\gamma$. The set K will be formed by the union of two parts: one is obtained from the optimal lower bound (2.3), while the other will come from a precise construction detailed below. Then the first part is given by

$$\lambda \geqslant \psi_1(d) = \frac{1}{2\alpha}\left(2\alpha^2 + (d - \alpha^2)S_1 - \sqrt{(2\alpha^2 + (d - \alpha^2)S_1)^2 - 4d\alpha^2}\right)$$

and

$$\lambda \leqslant \varphi_1(d) = \frac{1}{2\alpha}\left(2\alpha^2 + (d - \alpha^2)S_1 + \sqrt{(2\alpha^2 + (d - \alpha^2)S_1)^2 - 4d\alpha^2}\right),$$

with d belonging to the closed interval

$$I_1 = \left[\left(\frac{\alpha}{S_1}(2 - S_1) \right)^2, h_1^{\mathrm{I}}(\theta) a_2^{\mathrm{I}}(\theta) \right].$$

Then on the (d, λ)-plane the region is

$$K_1 = \left\{ (d, \lambda) \in \mathbb{R}_+^2 \quad \text{such that } d \in I_1 \text{ and } \psi_1(d) \leqslant \lambda \leqslant \varphi_1(d) \right\}.$$

First it is clear that φ_1 and ψ_1 are of class C^1 and that $\varphi_1(d)\psi_1(d) = d$. Calling

$$Ar(d) = (2\alpha^2 + (d - \alpha^2)S_1)^2 - 4d\alpha^2$$

we see that

$$\varphi_1''(d) = \frac{1}{2\alpha}\sqrt{Ar}'' = \frac{2ArAr'' - (Ar')^2}{8\alpha(Ar)^{3/2}} = \frac{-2\alpha^3(S_1 - 1)^2}{(Ar)^{3/2}} < 0.$$

Then $\varphi_1''(d) < 0$, so φ_1 is concave and ψ_1 is convex. One should notice that this curve is fully attained by rank-two laminates, more specifically they come from an iterated lamination with the isotropic phase, only if the restriction $\theta \geqslant \theta_{\min}^{\mathrm{I}}$ is met. If that restriction is not satisfied we close the region on the side of the bad conductors by doing one more lamination of the material on the curve with the least determinant with its rotation by $\pi/2$, and then we will have only part of the interval I_1, but still the same functions of the determinant, so the respective convexity and concavity will still hold.

The second part of K will come from the following construction: we first laminate $\mathbf{A}$ with $\mathbf{B}$ in the direction e_1 and using $\mathbf{A}$ in proportion η and $\mathbf{B}$ in proportion $1 - \eta$, to produce an intermediate diffusion tensor denoted by $\mathbf{M}_1$ and then laminate, in the direction of e_2, this tensor with the rotation of $\mathbf{B}$ by $\pi/2$, which we denote by $\tilde{\mathbf{B}}$, in proportions θ/η and $1-\theta/\eta$, respectively, with $\eta \in [\theta, 1]$. Then

$$\mathbf{M}_1 = \begin{bmatrix} h_1^{\mathrm{I}}(\eta) & 0 \\ 0 & a_2^{\mathrm{I}}(\eta) \end{bmatrix}$$

and then

$$\mathbf{M}_2(\eta) = \begin{bmatrix} \frac{\theta}{\eta} h_1^{\mathrm{I}}(\eta) + \left(1 - \frac{\theta}{\eta}\right)\gamma & 0 \\ 0 & \frac{\eta\beta a_2^{\mathrm{I}}(\eta)}{\theta\beta + (\eta-\theta)a_2^{\mathrm{I}}(\eta)} \end{bmatrix}.$$

We turn now to show that the corresponding functions φ_2 and ψ_2 are concave and convex, respectively, verification that will use that α is less than both β and γ, i.e. that the tensors are well-ordered. We will show that there is a value $\eta_0 \in (\theta, 1)$ where the determinant of $\mathbf{M}_2$ is maximized and then only the interval $[\eta_0, 1]$ will be used to define $\mathscr{L}_\theta$. To close the region on the side of the good conductors we laminate $\mathbf{M}_2(\eta_0)$ with its rotation by $\pi/2$. If the tensors are badly-ordered we did not get an analytical proof that the hypothesis of Proposition 3.4 are met, instead we computed a simple numerical approximation of the corresponding second derivatives, and verified that they always have the right sign for $\theta \in (0,1)$, $\alpha = 1$, $\gamma = 5$ and $\beta \in (0.2, 5)$.

Let us first define the following auxiliary functions of η: $A(\eta) = \alpha + \eta(\beta - \alpha)$ and $C(\eta) = \gamma - \eta(\gamma - \alpha)$, then we can write that the eigenvalue of $\mathbf{M}_2$ associated to e_1 is given by

$$\lambda_1 = g_1(\eta) = \frac{1}{\eta A}((\eta - \theta)\gamma A + \theta\alpha\beta)$$

and analogously

$$\lambda_2 = g_2(\eta) = \frac{\eta\beta C}{\theta\beta + (\eta - \theta)C},$$

both for $\eta \in [\theta, 1]$. Then

$$g_1'(\eta) = \frac{\theta}{\eta^2 A^2}(\alpha^2(\gamma - \beta) + 2\alpha\eta(\beta - \alpha)(\gamma - \beta) + \gamma\eta^2(\beta - \alpha)^2),$$

which is strictly positive, due to the well-ordering assumption,

$$g_1''(\eta) = \frac{-2\theta}{\eta^3 A^3}(\alpha^3(\gamma - \beta) + 3\alpha^2\eta(\beta - \alpha)(\gamma - \beta) + 3\alpha\eta^2(\beta - \alpha)^2(\gamma - \beta) + \gamma\eta^3(\beta - \alpha)^3),$$

which is strictly negative, again due to the well-order assumption, and

$$g_2'(\eta) = \frac{\theta\beta}{(\theta\beta + (\eta - \theta)C)^2}(-\gamma(\gamma - \beta) + 2\eta(\gamma - \beta)(\gamma - \alpha) - \eta^2(\gamma - \alpha)^2),$$

which is also strictly negative for $\eta \in [\theta, 1]$.

Let us now call $g_3(\eta) = g_1(\eta)g_2(\eta)$, we then have that $d = \lambda_1\lambda_2 = g_3(\eta)$ and one can show that

$$g_3'(\eta) = \theta\beta^2(\beta\gamma - \alpha^2)\frac{P(\eta)}{Q(\eta)},$$

where

$$P(\eta) = \theta\alpha(\gamma - \beta) + \eta^2(\gamma(\beta - \alpha) - \alpha(\gamma - \alpha) + \theta(\beta - \alpha)(\gamma - \alpha)) - 2\eta^3(\beta - \alpha)(\gamma - \alpha)$$

and

$$Q(\eta) = A^2(\theta\beta + (\eta - \theta)C)^2,$$

which is strictly positive for all $\eta \in (\theta, 1)$.

Now we see that P has two critical points, one at zero and the other one at

$$\eta_1 = \frac{1}{3}\left(\theta + \frac{\gamma(\beta - \alpha) - \alpha(\gamma - \alpha)}{(\beta - \alpha)(\gamma - \alpha)}\right).$$

Also we can see that P has only one positive real root, which we denote by η_0, and that lies in the interval $[\theta, 1]$ since

$$P(\theta) = \theta(1 - \theta)(\alpha(\gamma - \beta)(1 + \theta) + \theta^2(\gamma - \alpha)(\beta - \alpha)) > 0$$

and

$$P(1) = -(1 - \theta)(\beta\gamma + \alpha^2 - 2\alpha\beta) < 0.$$

Looking at the three cases: $\eta_1 < 0$, $\eta_1 = 0$ or $\eta_1 > 0$, we conclude that in all of them and once more using the well ordering of the original diffusion tensors, we will have that $g_3'(\eta) < 0$ for $\eta \in (\eta_0, 1]$ making then g_3 a bijection between $[\eta_0, 1]$ and $[g_3(1), g_3(\eta_0)]$.

Additionally, since

$$g_3''(\eta) = \frac{\theta\beta^2(\beta\gamma - \alpha^2)}{Q^2}(P'Q - PQ'),$$

and $P'(\eta_0) < 0$, we have that $g_3''(\eta_0) < 0$ and we will show that $(P'Q - PQ')' < 0$ for all $\eta \in (\eta_0, 1)$, which then will imply that $g_3''(\eta) < 0$ for all $\eta \in (\eta_0, 1)$, inequality that will be used later on,

$$(P'Q - PQ')' = P''Q - PQ'' < 0 \iff \frac{P''}{P} > \frac{Q''}{Q},$$

but $P''(\eta) < 0$ for $\eta \in (\eta_0, 1)$ and

$$Q''(\eta) = 2(\gamma(\beta - \alpha) - \alpha(\gamma - \alpha) + \theta(\beta - \alpha)(\gamma - \alpha)) - 6\eta(\beta - \alpha)(\gamma - \alpha),$$

which is negative for any $\eta > \eta_1$. But one can see that always $\eta_1 < \eta_0$, then we have for $\eta \in (\eta_0, 1)$ that $Q''(\eta) < 0$ and then for $\eta \in (\eta_0, 1)$ we get that

$$\frac{P''}{P} > 0 > \frac{Q''}{Q}.$$

Now on the interval $(\eta_0, 1)$ g_3 is a one-to-one C^1 function and then, by the inverse function theorem, g_3^{-1} is also C^1, therefore we have that $\eta = g_3^{-1}(d)$, hence we now define

$$\lambda_1 = \varphi_2(d) = g_1(g_3^{-1}(d)) \quad \text{and} \quad \lambda_2 = \psi_2(d) = g_2(g_3^{-1}(d)).$$

Then

$$\varphi_2'(d) = g_1'(g_3^{-1}(d))\frac{1}{g_3'(g_3^{-1}(d))},$$

and then, since g_1', g_2' are never zero, we can define

$$h_1(d) = \frac{1}{\varphi_2'(d)} = \left[\left(g_2 + g_2'\frac{g_1}{g_1'}\right) \circ g_3^{-1}\right](d),$$

analogously we also define

$$h_2(d) = \frac{1}{\psi_2'(d)} = \left[\left(g_1 + g_1'\frac{g_2}{g_2'}\right)\circ g_3^{-1}\right](d).$$

Now, in the context of Theorem 3.1, we set $\delta_1 = h_1^{\mathrm{I}}(\theta)a_2^{\mathrm{I}}(\theta) = g_3(1)$ and $\delta_2 = g_3(\eta_0)$. Then the first and fourth conditions of the Theorem easily hold and we only need to check the second and third conditions. But

$$\varphi_2''(d) < 0 \iff h_1'(d) > 0 \iff \left(\frac{g_3'}{g_1'}\right)' < 0 \iff \frac{g_3''}{g_3'} > \frac{g_1''}{g_1'},$$

which holds since the quantity on the left is positive and the quantity on the right is negative. Then φ_2 is concave.

Now

$$\psi_2''(d) > 0 \iff h_2'(d) < 0 \iff \left(\frac{g_3'}{g_2'}\right)' > 0 \iff g_1'' + 2\frac{g_1'g_2'}{g_2} < \frac{g_1'g_2''}{g_2'}.$$

But if at some point $\eta_2 \in (\eta_0, 1)$ the condition on the right would not hold, then at that point we would have that

$$\frac{g_2''}{g_1''g_2^2 + 2g_1'g_2g_2'} \leqslant \frac{g_2'}{g_1'g_2^2},$$

but on the other hand from $g_3''(\eta_2) < 0$ we conclude, also at η_2 that

$$\frac{g_2''}{g_1''g_2^2 + 2g_1'g_2g_2'} > \frac{-1}{g_1g_2},$$

then combining these two inequalities, we would have that at η_2

$$g_3'(\eta_2) > 0,$$

which is impossible and then ψ_2 is convex. Then we have that

$$K_2 = \left\{(d,\lambda) \in \mathbb{R}_+^2 : d \in [h_1^{\mathrm{I}}(\theta)a_2^{\mathrm{I}}(\theta), g_3(\eta_0)] \text{ and } \psi_2(d) \leqslant \lambda \leqslant \varphi_2(d)\right\}$$

and then we conclude that $K = K_1 \cup K_2$ gives $\mathscr{L}_\theta = \mathscr{M}(K)$ being H-stable, which is accomplished using Proposition 3.4.

3.3. Case II

Just like in case I, the part of the region coming from the optimal bound using rank-two laminates puts a restriction on θ, but it does not offer any difficulty on the verification of the hypothesis of Proposition 3.4, since it is obtained from the optimal upper bound (2.4) and is given by

$$\lambda \geqslant \psi_3(d) = \frac{1}{2\gamma}\left(\gamma^2 S_2 + d(2 - S_2) - \sqrt{(\gamma^2 S_2 + d(2 - S_2))^2 - 4d\gamma^2}\right)$$

and

$$\lambda \leqslant \varphi_3(d) = \frac{1}{2\gamma}\left(\gamma^2 S_2 + d(2 - S_2) + \sqrt{(\gamma^2 S_2 + d(2 - S_2))^2 - 4d\gamma^2}\right),$$

with d belonging to the closed interval

$$I_2 = \left[h_1^{\mathrm{II}}(\theta) a_2^{\mathrm{II}}(\theta), \left(\frac{\gamma S_2}{2 - S_2} \right)^2 \right].$$

Then on the (d, λ)-plane we call the region

$$L_1 = \left\{ (d, \lambda) \in \mathbb{R}_+^2 \quad \text{such that } d \in I_2 \text{ and } \psi_3(d) \leqslant \lambda \leqslant \varphi_3(d) \right\}.$$

The attainability of this bounding curve uses the restriction that $\theta \leqslant \theta_{\max}^{\mathrm{II}}$, but like in case I if that restriction is not satisfied, we will have only part of the interval I_2, but still the same functions, so the respective convexity and concavity will still hold.

We now show the way in which the second part of L is obtained: we first laminate $\mathbf{A}$ with $\mathbf{B}$ in the direction e_1 and using $\mathbf{A}$ in proportion η and $\mathbf{B}$ in proportion $1 - \eta$, to produce an intermediate diffusion tensor denoted $\mathbf{N}_1$ and then we make a laminate of this tensor with the rotation of $\mathbf{A}$ by $\pi/2$, which we denote by $\widetilde{\mathbf{A}}$, in the direction of e_2 and in proportions $\frac{1-\theta}{1-\eta}$ and $\frac{\theta-\eta}{1-\eta}$, respectively, with $\eta \in (0, \theta)$. Then

$$\mathbf{N}_1 = \begin{bmatrix} h_1^{\mathrm{II}}(\eta) & 0 \\ 0 & a_2^{\mathrm{II}}(\eta) \end{bmatrix}$$

and

$$\mathbf{N}_2(\eta) = \begin{bmatrix} \dfrac{\theta - \eta}{1 - \eta}\beta + \dfrac{1 - \theta}{1 - \eta} h_1^{\mathrm{II}}(\eta) & 0 \\ 0 & \dfrac{(1 - \eta)\alpha a_2^{\mathrm{II}}(\eta)}{(1 - \theta)\alpha + (\theta - \eta) a_2^{\mathrm{II}}(\eta)} \end{bmatrix}.$$

For this part of the boundary curve, like in the case I badly-ordered, we did not get an analytical proof that it satisfies the hypothesis of Proposition 3.4, so we also turned to a numerical verification, to check that the relevant second derivatives always have the right sign, which did happen for $\theta \in (0, 1)$, $\alpha = 1$, $\gamma = 5$ and $\beta \in (1, 25)$.

4. Comparing $\mathscr{G}_\theta$, or $\widetilde{\mathscr{G}}_\theta$, with $\mathscr{L}_\theta$

When the restriction on the volume fraction imposed by Theorem 2.1 or 2.2, either $\theta \geqslant \theta_{\min}^{I}$ in case I or $\theta \leqslant \theta_{\max}^{\mathrm{II}}$ in case II, is not satisfied, the corresponding bound is most likely non-optimal because, for example in case I taking $\theta \approx 0$ and $\beta \approx \alpha$, we will have $S_1 \approx 1$ and then the right hand side of (2.3) goes to infinity, which will then force an isotropic material saturating the bound, to have conductivity very close to α, which seems not to be attainable since we will be mixing a very low proportion of the isotropic material αI with a very high proportion of a material like $\mathrm{diag}(\alpha, \gamma)$. Besides the worst isotropic conductor in $\mathscr{L}_\theta$ will have conductivity close to $\sqrt{\alpha\gamma}$ and then the relative difference between this and the isotropic material sitting on the bounding curve should be like

$$\frac{\sqrt{\gamma} - \sqrt{\alpha}}{\sqrt{\alpha}},$$

which can be made as big as desired, by playing with α or γ. Therefore on the side of the region close to the isotropic phase we either have no gap between $\mathscr{L}_\theta$ and either $\mathscr{G}_\theta$ or $\widetilde{\mathscr{G}}_\theta$, if the constraint on θ holds, or in the opposite case, the gap between them can be very big, most likely due to the non-optimality of the bound.

Therefore to compare the two regions we focus only on the gap on the side of the region closer to the anisotropic phase. For case I in Fig. 1 we fix $\alpha = 1$ and $\gamma = 5$ and make a fine discretization of θ and β and draw the contour plot of the function of these two variables given by the percentage of the conductivity of

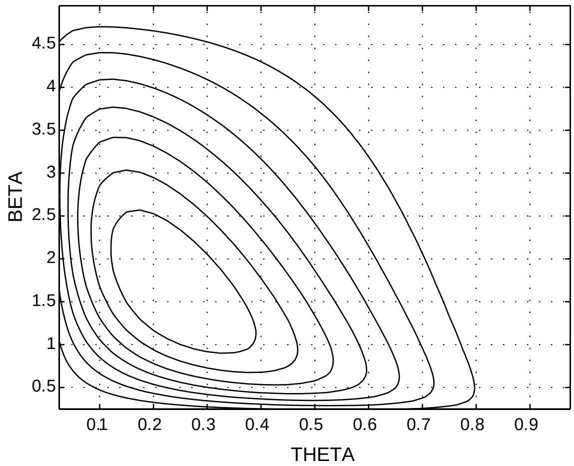

Fig. 1. Case I: $\alpha = 1$ and $\gamma = 5$.

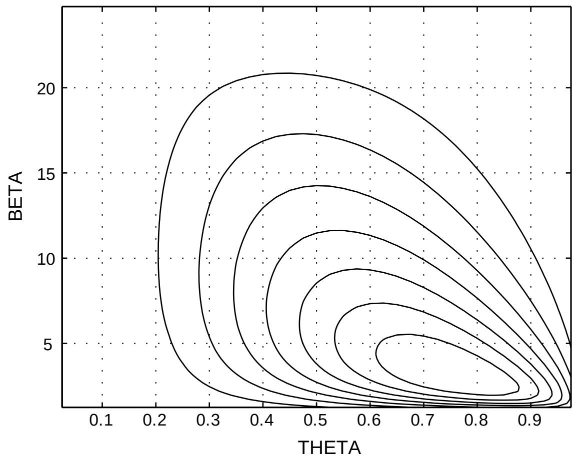

Fig. 2. Case II: $\alpha = 1$ and $\gamma = 5$.

the best isotropic conductor in $\widetilde{\mathscr{G}}_\theta$, represented by the difference between that conductivity and the conductivity of the best isotropic conductor in $\mathscr{L}_\theta$. For the quantity mentioned before the last, one has an explicit formula, but for the last one we do not have an explicit formula. The maximum value in this graph is of 2.07%, which is attained for $\theta = 0.23$ and $\beta = 1.69$.

For case II in Fig. 2 we present the analogous plot. The maximum value in this graph is of 2.11%, which is attained for $\theta = 0.75$ and $\beta = 3.16$.

In both cases we see that the gap is quite small for most combinations of θ and β, the gap being of about 2% only for something like 5% of such combinations.

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