BOUNDS ON THE EFFECTIVE BEHAVIOR OF A SQUARE CONDUCTING LATTICE

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Abstract

A collection of resistors with two possible resistivities is considered. This paper investigates the overall or macroscopic behavior of a square two–dimensional lattice of such resistors when each type is present in fixed proportion in the lattice. The macroscopic behavior is that of an anisotropic conductor at the continuum level and the goal of the paper is to describe the set of all possible such conductors. This is thus a problem of bounds in the footstep of an abundant literature on the topic in the continuum case. The originality of the paper is that the investigation focusses on the interplay between homogenization and the passage from a discrete network to a continuum. A set of bounds is proposed and its optimality is shown when the proportion of each resistor on the discrete lattice is $\frac{1}{2}$. We conjecture that the derived bounds are optimal for all proportions.

Keywords: Γ–convergence, lattice, resistor network, homogenization, bounds, optimality.

1 Introduction

The derivation of bounds on the effective behavior of a mixture of two isotropic conductors in fixed volume fraction has a long history. It originates in the elementary so–called Voigt & Reuss harmonic–arithmetic bounds on the possible conductivity tensors A, that is

$$\underline{a}(\theta)|\xi|^2 \le \langle A\xi, \xi\rangle \le \overline{a}(\theta)|\xi|^2, \xi \in \mathbb{R}^N$$

with

$$\frac{1}{\underline{a}(\theta)} := \frac{\theta}{\alpha} + \frac{1-\theta}{\beta};\ \overline{a}(\theta) := \theta\alpha + (1-\theta)\beta,$$

where we denote by α and β the conductivity of the core conductors and by θ the proportion of the α–conductor, and it culminates in the derivation by Murat & Tartar of optimal bounds for all conductivity tensors resulting from such mixtures: see [11]; see also the derivation of Cherkaev & Lurie in the two–dimensional case [6]. The (two–dimensional) optimal bounds only constrain the eigenvalues λ_1, λ_2 of the macroscopic conductivity tensor A. The formula is

$$\begin{cases} \dfrac{1}{\lambda_1-\alpha} + \dfrac{1}{\lambda_2-\alpha} \le \dfrac{1}{\overline{a}(\theta)-\alpha} + \dfrac{1}{\underline{a}(\theta)-\alpha} \\[2ex] \dfrac{1}{\beta-\lambda_1} + \dfrac{1}{\beta-\lambda_2} \le \dfrac{1}{\beta-\overline{a}(\theta)} + \dfrac{1}{\beta-\underline{a}(\theta)}. \end{cases} \tag{1.1}$$

A great variety of constitutive behaviors has been subsequently analyzed resulting in a long list of bounds on various binary or multiphase mixtures of materials exhibiting those constitutive behaviors. Since most of the available mathematical methods used in such analyses derive form the mathematical notion of G– or H–convergence (see e.g. [8]), the problem of deriving those bounds has been assigned the generic name of G–closure problem in the mathematical literature. The interested reader is invited to consult the mammoth encyclopaedia [7] and references therein. But, in fact, two–phase isotropic conductivity is the only complete success of the available bounding methods as of yet.

In an apparently different direction, the derivation of continuum models from discrete lattice models has an even longer history. At the beginning of the XIX$^{\text{th}}$ century, CAUCHY deduced a first model for isotropic linear elasticity from a lattice of springs, his derivation constraining the POISSON's ratio ν to equal $\frac{1}{4}$. The model was later improved by MAXWELL and generalized to arbitrary $\nu \in (-1, \frac{1}{2})$. In solid state physics, it has become customary to introduce an atomic lattice and to postulate or argue in favor of an interatomic interaction potential as a means for deriving suitable macroscopic behaviors. In truth, the mathematical formalization of such an approach has been slow to emerge for a lack of appropriate mathematical tools.

Whenever inertia effects are neglected — an admittedly challengeable assumption — the passage from discrete models to a continuum may be conveniently framed in a variational (energetic) framework, that of Γ–convergence, first introduced by DE GIORGI. We do not recall the definition here but refer e.g. to [2] for a simple introduction to the topic, or to the compendium [3]. In that approach, the discrete energies associated to an energy minimizing configuration for the lattice in a given volume under well–suited boundary conditions on the boundary of that volume are shown to converge to the continuum energy associated to an energy minimizing configuration for the continuum model under those same boundary conditions. We refer to [1] and references therein.

In the present study, we attempt to investigate, on a decidedly over–simplistic model, the link between lattice mixing and macroscopic behavior. Specifically, we consider the simplest available model, that of a square two–dimensional lattice of resistors. If all resistors have the same resistivity α, then it is a simple matter to show (through e.g. Γ–convergence) that the corresponding continuum will be a linear isotropic conductor with conductivity α. We propose to examine the equivalent of the bounding problem evoked at the onset of this introduction, that is the lattice mixing of two resistivities α and β with given proportion θ of resistivity α. A first, and misguided, intuition would lead one to the conclusion that, since a square lattice with resistivity α gives rise to an isotropic conductor with conductivity α, the proposed mixture will give rise to a conductivity tensor which can be obtained as a mixture in volume fraction $\theta, 1-\theta$ of α and β conductors. Thus, the resulting conductivity tensor should have eigenvalues that lie in the set defined by (1.1). Such is not the case and the resulting set of conductors is much larger (see Theorem 4.2 and the concluding remarks). In Fig. 1 we picture the two-dimensional sets of eigenvalues (λ_1, λ_2) corresponding to diagonal matrices in the two situations.

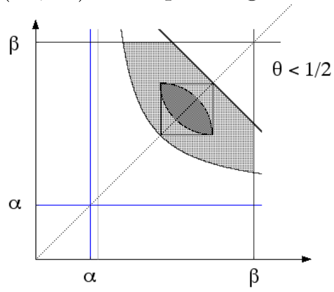

Figure 1: comparison of bounds

In truth, the problem seen as a mixture of continua, is more akin to that of a mixture of three conductors, two being isotropic with conductivities α and β, one being anisotropic with conductivity $\begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix}$ in a fixed basis of $\mathbb{R}^2$. The volume fractions of each material $\theta_1, \theta_2, \theta_3$ with $\theta_1 + \theta_2 + \theta_3 = 1$ should be such that the total volume fraction of α is θ, i.e., $\theta_1 + \frac{1}{2}\theta_2 = \theta$.

In any case, in this paper we derive bounds on the set of macroscopic conductivities (Theorem 4.2, Proposition 5.1) and show those to be optimal in the case $\theta = \frac{1}{2}$ (see Theorem 6.1) and for all macroscopic conductivity tensors that are diagonal in the lattice basis (see Theorem 4.2). We conjecture in the concluding remarks that the obtained bounds are always optimal, although such optimality in the case $\theta \neq \frac{1}{2}$ has only been obtained for the 'mid–matrix' as explained in those remarks.

As a final note, our result could be interpreted as some weak challenge to the conceptual validity of bounds derived purely at the continuum level, provided of course that one trusts the discrete to continuum approach to be a reasonable one, at least as far as crystalline solids are concerned.

2 A G-closure problem

Let Ω be a bounded open subset of $\mathbb{R}^2$ with Lipschitz boundary. For every fixed $\varepsilon > 0$ and any open subset $U \subset \Omega$ we consider the quadratic discrete energy

$$F_\varepsilon(u,U) = \frac{1}{2}\sum_{i,j} c^\varepsilon_{ij}(u_i - u_j)^2 \tag{2.1}$$

defined on all functions $u : \varepsilon\mathbb{Z}^2 \cap \Omega \to \mathbb{R}$. The sum is performed on 'nearest neighbours'; i.e., points $i, j \in \varepsilon\mathbb{Z}^2 \cap U$ such that $|i-j| = \varepsilon$, and we write $u_i = u(i)$. It is clearly not restrictive to suppose that $c^\varepsilon_{ij} = c^\varepsilon_{ji}$. It is often convenient to rewrite this energy as

$$F_\varepsilon(u,U) = \sum_i h^\varepsilon_i (u_{(i_1+1,i_2)} - u_{(i_1,i_2)})^2 + \sum_i v^\varepsilon_i (u_{(i_1,i_2+1)} - u_{(i_1,i_2)})^2, \tag{2.2}$$

where $h^\varepsilon_i = c^\varepsilon_{i,i+e_1}$, $v^\varepsilon_i = c^\varepsilon_{i,i+e_2}$, thus separating the 'horizontal' and 'vertical' interactions.

If the coefficients c^ε_{ij} are equibounded, thanks to general compactness results (see [12], [9], Propositions 2.6 and 2.15, [1], Theorems 3.2, 3.3), we can let $\varepsilon \to 0$ and obtain, upon passing to a subsequence (independent of U), a quadratic energy of the form

$$F_0(u,U) = \int_U \langle A(x)Du, Du\rangle\, dx \tag{2.3}$$

defined on $H^1(U)$ as a Γ-limit.

In this paper we face the problem of the description of all possible such F_0 when we suppose that $c^\varepsilon_{ij} \in \{\alpha,\beta\}$, where $0 < \alpha \le \beta$ are two fixed positive numbers, and we fix the proportion of nearest neighbours such that $c^\varepsilon_{ij} = \alpha$ (and as a consequence of those such that $c^\varepsilon_{ij} = \beta$).

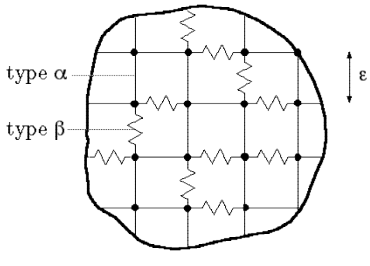

Figure 2: a square network

A particular case is when the coefficients c^ε_{ij} are obtained by scaling a fixed periodic function; i.e., there exists $N \in \mathbb{N}$ and periodic functions $h, v : \mathbb{Z}^2 \to \{\alpha,\beta\}$ periodic of period N in both arguments such that

$$h^\varepsilon_i = h\Big(\frac{i}{\varepsilon}\Big), \qquad v^\varepsilon_i = v\Big(\frac{i}{\varepsilon}\Big). \tag{2.4}$$

In this case the matrix A is independent of x and is given by the *homogenization formula* ([1], Theorem 4.1):

$$\langle A\xi,\xi\rangle \quad = \quad \frac{1}{N^2}\min\Big\{\sum_{i\in\{1,\dots,N\}^2} h_i(\xi_1 + \varphi(i_1+1,i_2) - \varphi(i_1,i_2))^2$$

$$+\sum_{i\in\{1,\dots,N\}^2} v_i(\xi_2+\varphi(i_1,i_2+1)-\varphi(i_1,i_2))^2 :$$
$$\varphi:\mathbb{Z}^2\to\mathbb{R}\ N\text{-periodic}\Big\} \tag{2.5}$$

Note that the particular cases c^ε_{ij} identically equal to α or β give $A=\alpha I$ and βI respectively.

If $\theta\in\mathbb{Q}\cap[0,1]$ we then define $\mathcal{H}(\theta)$ as the set of matrices given by (2.5) and such that

$$\theta=\frac{1}{2N^2}(\#\{i\in\{1,\dots,N\}^2 : h_i=\alpha\}+\#\{i\in\{1,\dots,N\}^2 : v_i=\alpha\}); \tag{2.6}$$

i.e., the proportion of α-connections is θ (and hence that of β-connections is $1-\theta$). The definition of $\mathcal{H}(\theta)$ is extended to $\theta\in[0,1]$ by continuity.

If the coefficients are not periodic, we can describe the *local proportion* $\theta(x)$ of α-connections by

$$\theta(x)=\lim_{\rho\to0}\lim_{\varepsilon\to0}\frac{\#\{i\in\varepsilon\mathbb{Z}^2\cap Q_\rho(x) : h^\varepsilon_i=\alpha\}+\#\{i\in\varepsilon\mathbb{Z}^2\cap Q_\rho(x) : h^\varepsilon_i=\alpha\}}{2\#\{i\in\varepsilon\mathbb{Z}^2\cap Q_\rho(x)\}}, \tag{2.7}$$

where $Q_\rho(x)$ is the coordinate cube centered at x and with side length ρ. Note that this quantity is well defined for $x\in\Omega\setminus N$, upon extraction of a subsequence in ε, where $|N|=0$. Further, $\int_\Omega\theta\,dx$ represents the total proportion of α-connections.

Once such θ is defined the matrices A are characterized by a *localization principle* ([11], [4], [10]).

Proposition 2.1 *$A(x)\in\mathcal{H}(\theta(x))$ for almost all $x\in\Omega$.*

Proof. We only sketch the main points of the proof. Let $\overline{x}$ be a Lebesgue point for $\theta(x)$. Upon a translation argument we can suppose that $\overline{x}=0$. For all open sets U the functional $\int_U\langle A(0)Du,Du\rangle\,dx$ is the Γ-limit of $\int_U\langle A(\rho x)Du,Du\rangle\,dx$ as $\rho\to0$ since $A(\rho x)$ converges to $A(0)$ in L^1 on U. We can then infer that, for any fixed ξ,

$$\langle A(\overline{x})\xi,\xi\rangle=\min\Big\{\int_{Q_1(0)}\langle A(\rho x)(\xi+D\varphi),(\xi+D\varphi)\rangle : \varphi\ 1\text{-periodic}\Big\}+o(1) \tag{2.8}$$

as $\rho\to0$. We now remark that the passage from discrete to continuous is independent of the specific (well chosen) boundary condition, or still that the Γ–convergence result holds true as well if periodic boundary conditions are imposed on $\partial Q_{1/\rho}(0)$ (see [1], Theorem 3.12), which implies that

$$\begin{aligned}&\min\{\int_{Q_1(0)}\langle A(\rho x)(\xi+D\varphi),(\xi+D\varphi)\rangle : \varphi\ 1\text{-periodic}\}\\ =\ &\rho^2\min\{F_0(\xi+D\varphi,Q_{1/\rho}(0)) : \varphi\ 1/\rho\text{-periodic}\}\\ =\ &\lim_{\varepsilon\to0}\rho^2\min\{F_\varepsilon(\xi+D\varphi,Q_{1/\rho}(0)) : \varphi\ 1/\rho\text{-periodic}\}.\end{aligned} \tag{2.9}$$

We may suppose that $N=1/\rho\in\mathbb{N}$, so that the formula in the last limit is of the type (2.5) for some θ_ρ tending to $\theta(\overline{x})$ as $\rho\to0$, and the proposition is proved.

The previous proposition reduces the problem of characterizing all $A(x)$ to that of studying the sets $\mathcal{H}(\theta)$ for fixed $\theta\in[0,1]$, which is precisely the subject of the remainder of this work.

3 Trivial bounds

We denote by $\mathcal{H}(\theta_h,\theta_v)$ those matrices in $\mathcal{H}(\theta)$ with fixed volume fraction θ_h,θ_v of horizontal/vertical α-connections; i.e., for $\theta_h,\theta_v\in\mathbb{Q}$,

$$\theta_h=\frac{1}{N^2}\#\{i\in\{1,\dots,N\}^2 : h_i=\alpha\}, \tag{3.1}$$
$$\theta_v=\frac{1}{N^2}\#\{i\in\{1,\dots,N\}^2 : v_i=\alpha\}. \tag{3.2}$$

Note that

$$\theta_h + \theta_v = 2\theta, \tag{3.3}$$

so that we have

$$\begin{aligned}
\mathcal{H}(\theta) &= \bigcup\{\mathcal{H}(t, 2\theta - t) : 0 \le t \le 1, 0 \le 2\theta - t \le 1\} \\
&= \begin{cases} \bigcup\{\mathcal{H}(t, 2\theta - t) : 0 \le t \le 2\theta\} & \text{if } 0 \le \theta \le 1/2 \\ \bigcup\{\mathcal{H}(t, 2\theta - t) : 1 - 2\theta \le t \le 1\} & \text{if } 1/2 \le \theta \le 1. \end{cases}
\end{aligned} \tag{3.4}$$

We define the harmonic and arithmetic means of α and β in proportion $s, 1 - s$ to be

$$\underline{a}(s) = \frac{\alpha\beta}{s\beta + (1 - s)\alpha}, \qquad \overline{a}(s) = s\alpha + (1 - s)\beta,$$

respectively. Note that

$$\frac{1}{\underline{a}(\theta_h)} + \frac{1}{\underline{a}(\theta_v)} = \frac{2}{\underline{a}(\theta)}, \qquad \overline{a}(\theta_h) + \overline{a}(\theta_v) = 2\overline{a}(\theta). \tag{3.5}$$

Let $A \in \mathcal{H}(\theta_h, \theta_v)$ be given by (2.5). By testing with $\varphi = 0$ in (2.5) we get

$$\langle A\xi, \xi\rangle \le \frac{1}{N^2}\Big(\sum_{i \in \{1,\dots,N\}^2} h_i\xi_1^2 + \sum_{i \in \{1,\dots,N\}^2} v_i\xi_2^2\Big) = \overline{a}(\theta_h)\xi_1^2 + \overline{a}(\theta_v)\xi_2^2. \tag{3.6}$$

Conversely, for all φ, the convexity of $(x, y) \to \dfrac{y^2}{x}$ for positive x's yields

$$\begin{aligned}
&\frac{1}{N^2}\Big(\sum_{i \in \{1,\dots,N\}^2} h_i(\xi_1 + \varphi(i_1 + 1, i_2) - \varphi(i_1, i_2))^2 \\
&\qquad + \sum_{i \in \{1,\dots,N\}^2} v_i(\xi_2 + \varphi(i_1, i_2 + 1) - \varphi(i_1, i_2))^2\Big) \\
&= \frac{1}{N^2}\sum_{i_2=1}^{N}\sum_{i_1=1}^{N} h_i(\xi_1 + \varphi(i_1 + 1, i_2) - \varphi(i_1, i_2))^2 \qquad (3.7)\\
&\qquad + \frac{1}{N^2}\sum_{i_1=1}^{N}\sum_{i_2=1}^{N} v_i(\xi_2 + \varphi(i_1, i_2 + 1) - \varphi(i_1, i_2))^2 \\
&\ge \frac{1}{N}\sum_{k=1}^{N}\underline{a}(\theta_h^k)\xi_1^2 + \frac{1}{N}\sum_{k=1}^{N}\underline{a}(\theta_v^k)\xi_2^2, \qquad (3.8)
\end{aligned}$$

where

$$\theta_h^k = \frac{1}{N}\#\{i_1 : h_{(i_1,k)} = \alpha\}, \qquad \theta_v^k = \frac{1}{N}\#\{i_2 : h_{(k,i_2)} = \alpha\}.$$

By the convexity of $\underline{a}$ and the arbitrariness of φ we immediately obtain

$$\underline{a}(\theta_h)\xi_1^2 + \underline{a}(\theta_v)\xi_2^2 \le \langle A\xi, \xi\rangle. \tag{3.9}$$

We obtain the 'trivial' estimates detailed in the following proposition.

Proposition 3.1 *If $A \in \mathcal{H}(\theta_h, \theta_v)$ then*

$$\underline{a}(\theta_h)\xi_1^2 + \underline{a}(\theta_v)\xi_2^2 \le \langle A\xi, \xi\rangle \le \overline{a}(\theta_h)\xi_1^2 + \overline{a}(\theta_v)\xi_2^2 \tag{3.10}$$

for all $\xi \in \mathbb{R}^2$.

4 Exact bounds for diagonal matrices

We denote by $\mathcal{H}_d(\theta)$, $\mathcal{H}_d(\theta_h,\theta_v)$ the set of diagonal matrices in $\mathcal{H}(\theta)$ and $\mathcal{H}(\theta_h,\theta_v)$, respectively.

The first observation is that for $A\in\mathcal{H}_d(\theta_h,\theta_v)$ the 'trivial' bounds are optimal. In particular we can obtain the 'extremal' matrices $\mathrm{diag}(\underline{a}(\theta_h),\underline{a}(\theta_v))$ and $\mathrm{diag}(\overline{a}(\theta_h),\overline{a}(\theta_v))$ that are obtained by placing all connections in series/parallel in both horizontal and vertical directions, a 'microstructure' which is not feasible in the continuous case.

Proposition 4.1 *We have*

$$\mathcal{H}_d(\theta_h,\theta_v)=\{\mathrm{diag}(x,y):\underline{a}(\theta_h)\le x\le\overline{a}(\theta_h),\underline{a}(\theta_v)\le y\le\overline{a}(\theta_v)\}.$$

Proof. It suffices to prove that $\mathrm{diag}(\underline{a}(\theta_h),\underline{a}(\theta_v)),\mathrm{diag}(\overline{a}(\theta_h),\overline{a}(\theta_v))\in\mathcal{H}_d(\theta_h,\theta_v)$, the construction for all other matrices following easily.

In order to obtain $\mathrm{diag}(\underline{a}(\theta_h),\underline{a}(\theta_v))$, let $\theta_h=M_1/N$, and $\theta_v=M_2/N$. We then define (see Fig. 3)

$$h_{(i_1,i_2)}=:h_{i_1}=\begin{cases}\alpha & \text{if } 1\le i_1\le M_1\\ \beta & \text{otherwise}\end{cases}, \tag{4.1}$$

$$v_{(i_1,i_2)}=:v_{i_2}=\begin{cases}\alpha & \text{if } 1\le i_2\le M_2\\ \beta & \text{otherwise}\end{cases}. \tag{4.2}$$

It is easily seen that (3.9) is sharp for this choice of h_i,v_i. Indeed, if ζ and ψ are the one-dimensional minimizers for

$$\frac{1}{N}\sum_i h_i(\xi_1+\varphi(i+1)-\varphi(i))^2 \tag{4.3}$$

and

$$\frac{1}{N}\sum_i v_i(\xi_2+\varphi(i+1)-\varphi(i))^2 \tag{4.4}$$

among all N–periodic φ's — for which the minimal values are respectively $\underline{a}(\theta_h)\xi_1^2$ and $\underline{a}(\theta_v)\xi_2^2$ — then $\zeta(i_1)+\psi(i_2)$ is a minimizer for (2.5) for the choice (4.1)–(4.2) for $h_{(i_1,i_2)}$ and $v_{(i_1,i_2)}$.

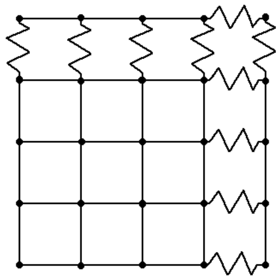

Figure 3: optimal network for harmonic means

Conversely, to obtain $\mathrm{diag}(\overline{a}(\theta_h),\overline{a}(\theta_v))$ it suffices to choose

$$h_{(i_1,i_2)}=:h_{i_1}=\begin{cases}\alpha & \text{if } 1\le i_2\le M_1\\ \beta & \text{otherwise}\end{cases},$$

$$v_{(i_1,i_2)}=:v_{i_2}=\begin{cases}\alpha & \text{if } 1\le i_1\le M_2\\ \beta & \text{otherwise}\end{cases}$$

(see Fig. 4). In that case, $\varphi\equiv 0$ is a minimizer because 0 is a minimizer of the one–dimensional problems (4.3),(4.4).

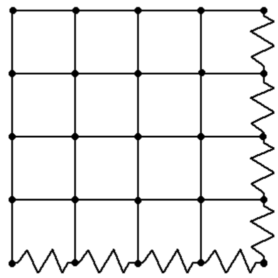

Figure 4: optimal network for arithmetic means

From Proposition 4.1 we immediately obtain the complete description of $\mathcal{H}_d(\theta)$.

Theorem 4.2 (exact bounds for diagonal matrices) *The set* $\mathcal{H}_d(\theta)$ *is composed of all matrices* $\mathrm{diag}(x, y)$ *satisfying*

(i) *(case* $0 \le \theta \le 1/2$*)* $\underline{a}(2\theta) \le x, y \le \beta$, $x + y \le 2\overline{a}(\theta)$, $\dfrac{1}{y} + \dfrac{1}{x} \le \dfrac{2}{\underline{a}(\theta)}$;

(ii) *(case* $1/2 \le \theta \le 1$*)* $\alpha \le x, y \le \overline{a}(2\theta - 1)$, $x + y \le 2\overline{a}(\theta)$, $\dfrac{1}{y} + \dfrac{1}{x} \le \dfrac{2}{\underline{a}(\theta)}$.

Note that for $\theta = 1/2$ then the form of the bounds simplify since $\underline{a}(2\theta) = \alpha$ and $\overline{a}(2\theta - 1) = \beta$. The shape of the set $\mathcal{H}_d(\theta)$ in the three cases is pictured in Fig. 5.

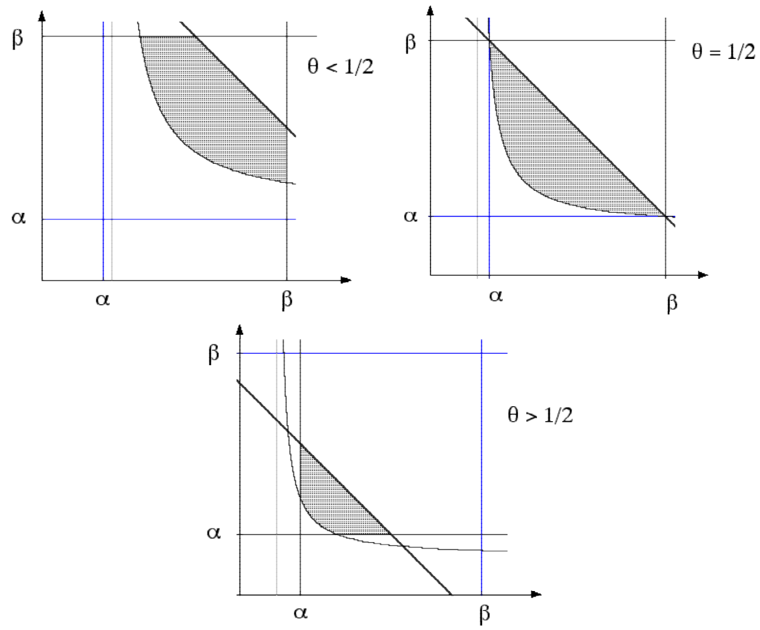

Figure 5: the sets $\mathcal{H}_d(\theta)$

Proof. The proof is an immediate consequence of Proposition 4.1, taking into account (3.5) and (3.4).

5 An outer bound for non-diagonal matrices

Let $A = \begin{pmatrix} x & z \\ z & y \end{pmatrix} \in \mathcal{H}(\theta_h, \theta_v)$. From the 'trivial' bounds we obtain

$$\underline{a}(\theta_h)\xi_1^2 + \underline{a}(\theta_v)\xi_2^2 \le \langle A\xi, \xi\rangle \le \overline{a}(\theta_h)\xi_1^2 + \overline{a}(\theta_v)\xi_2^2 \tag{5.1}$$

for all $\xi \in \mathbb{R}^2$. By testing with the vectors $(1,0)$ and $(0,1)$ we get

$$\underline{a}(\theta_h) \leq x \leq \overline{a}(\theta_h), \qquad \underline{a}(\theta_v) \leq y \leq \overline{a}(\theta_v), \tag{5.2}$$

i.e, $A_d = \begin{pmatrix} x & 0 \\ 0 & y \end{pmatrix} \in \mathcal{H}_d(\theta_h, \theta_v)$. That is, the projection of $\mathcal{H}(\theta_h, \theta_v)$ onto diagonal matrices is precisely $\mathcal{H}_d(\theta_h, \theta_v)$.

In general, we can obtain an estimate for the off-diagonal term z from (5.1) by optimizing the inequalities

$$(\underline{a}(\theta_h) - x)\xi_1^2 + (\underline{a}(\theta_v) - y)\xi_2^2 \leq 2z\xi_1\xi_2 \leq (\overline{a}(\theta_h) - x)\xi_1^2 + (\overline{a}(\theta_v) - y)\xi_2^2, \tag{5.3}$$

that gives

$$z^2 \leq \min\{(\overline{a}(\theta_h) - x)(\overline{a}(\theta_v) - y), (x - \underline{a}(\theta_h))(y - \underline{a}(\theta_v))\}. \tag{5.4}$$

We now fix $\theta \leq 1/2$ and maximize the range of values for z with respect to θ_h, θ_v with $\theta_h + \theta_v = 2\theta$ in the following two inequalities

$$z^2 \leq (\overline{a}(\theta_h) - x)(\overline{a}(\theta_v) - y) \tag{5.5}$$

$$z^2 \leq (x - \underline{a}(\theta_h))(y - \underline{a}(\theta_v)). \tag{5.6}$$

This computation will give us an analytic 'outer bound'.

By symmetry *we carry this computation for $x \leq y$ only.*

Bound from arithmetic means. We choose $\overline{a}(\theta_h)$ as independent variable. The constraint that $A \in \mathcal{H}(\theta_h, \theta_v)$ becomes, in terms of $\overline{a}(\theta_h)$,

$$\begin{cases} \dfrac{\alpha\beta}{\alpha + \beta - \overline{a}(\theta_h)} \leq x \leq \overline{a}(\theta_h) \\[2ex] \dfrac{\alpha\beta}{\alpha + \beta - 2\overline{a}(\theta) + \overline{a}(\theta_h)} \leq y \leq 2\overline{a}(\theta) - \overline{a}(\theta_h) \end{cases}$$

that is

$$\begin{cases} x \leq \overline{a}(\theta_h) \leq \alpha + \beta - \dfrac{\alpha\beta}{x} \\[2ex] 2\overline{a}(\theta) - (\alpha + \beta) + \dfrac{\alpha\beta}{y} \leq \overline{a}(\theta_h) \leq 2\overline{a}(\theta) - y \end{cases}.$$

Thus,

$$t_m(x,y) := \max\{x, 2\overline{a}(\theta) - (\alpha + \beta) + \frac{\alpha\beta}{y}\} \leq \overline{a}(\theta_h) \leq t_M(x,y) := \min\{2\overline{a}(\theta) - y, \alpha + \beta - \frac{\alpha\beta}{x}\}.$$

These two relations define three separate regions in $\mathcal{H}_d(\theta)$ bound by the non–intersecting curves

$$\begin{cases} x = 2\overline{a}(\theta) - (\alpha + \beta) + \dfrac{\alpha\beta}{y} \\[2ex] y = 2\overline{a}(\theta) - (\alpha + \beta) + \dfrac{\alpha\beta}{x}, \end{cases}.$$

two hyperbolae passing respectively through the two upper and two lower corner points of $\mathcal{H}_d(\theta)$.

Recall the relation

$$\overline{a}(\theta_h) + \overline{a}(\theta_v) = 2\overline{a}(\theta) \tag{5.7}$$

and compute

$$\begin{aligned} f_a(x,y) &= \max\{(\overline{a}(\theta_h)-x)(\overline{a}(\theta_v)-y) : \mathrm{diag}(x,y)\in\mathcal{H}(\theta_h,\theta_v)\} \\ &= \max\{(t-x)(2\overline{a}(\theta)-t-y) : t_m(x,y)\le t\le t_M(x,y)\}. \end{aligned} \tag{5.8}$$

That gives

$$f_a(x,y)=\begin{cases} \Big(\overline{a}(\theta)-\dfrac{x+y}{2}\Big)^2 \text{ if } x\ge 2(\overline{a}(\theta)-(\alpha+\beta))+y+2\dfrac{\alpha\beta}{y} \\ \\ (\alpha+\beta-(\dfrac{\alpha\beta}{y}+y))((1-2\theta)(\beta-\alpha)+\dfrac{\alpha\beta}{y}-x) \text{ otherwise.} \end{cases} \tag{5.9}$$

The maximum in (5.9) is reached for

$$\overline{a}(\theta_h)=\begin{cases} \overline{a}(\theta)+\frac{x-y}{2} & \text{if } x\ge 2(\overline{a}(\theta)-(\alpha+\beta))+y+2\dfrac{\alpha\beta}{y} \\ \\ 2\overline{a}(\theta)-(\alpha+\beta)+\dfrac{\alpha\beta}{y} & \text{otherwise.} \end{cases} \tag{5.10}$$

Bound from harmonic means. By choosing $\underline{a}(\theta_h)$ as independent variable, the constraint that $A\in\mathcal{H}(\theta_h,\theta_v)$ in terms of $\underline{a}(\theta_h)$ becomes

$$\begin{array}{rcl} \underline{a}(\theta_h)\le & x & \le \alpha+\beta-\dfrac{\alpha\beta}{\underline{a}(\theta_h)} \\ \dfrac{\underline{a}(\theta_h)\,\underline{a}(\theta_h)}{2\underline{a}(\theta_h)-\underline{a}(\theta)}\le & y & \le \alpha+\beta+\dfrac{\alpha\beta}{\underline{a}(\theta_h)}-\dfrac{2\alpha\beta}{\underline{a}(\theta)}, \end{array}$$

that can be summarized in $t_m(x,y)\le\underline{a}(\theta_h)\le t_M(x,y)$, where

$$\begin{aligned} t_m(x,y) &= \max\Big\{\frac{y\,\underline{a}(\theta)}{2y-\underline{a}(\theta)},\frac{\alpha\beta}{\alpha+\beta-x}\Big\}, \\ t_M(x,y) &= \min\Big\{\frac{\alpha\beta\,\underline{a}(\theta)}{\underline{a}(\theta)(y-(\alpha+\beta))+2\alpha\beta},x\Big\}, \end{aligned}$$

Note that the regions defined by these relations are the same as those defined in the case of the arithmetic means.

We can then compute

$$f_h(x,y):=\max\Big\{(x-t)\Big(y-\frac{\underline{a}(\theta)\,t}{2t-\underline{a}(\theta)}\Big) : t_m(x,y)\le t\le t_M(x,y)\Big\}. \tag{5.11}$$

Recalling the relation

$$\frac{1}{\underline{a}(\theta_h)}+\frac{1}{\underline{a}(\theta_v)}=\frac{2}{\underline{a}(\theta)}=\frac{1}{\underline{a}(2\theta)}+\frac{1}{\beta}, \tag{5.12}$$

we then obtain

$$f_h(x,y)=\begin{cases} \dfrac14\Big(\underline{a}(\theta)-\sqrt{(2x-\underline{a}(\theta))(2y-\underline{a}(\theta))}\Big)^2 \\ \quad\text{if } 2\alpha\beta(\alpha\beta+\underline{a}(\theta)(y-(\alpha+\beta)))(2x-\underline{a}(\theta))\le\underline{a}(\theta)^2(\alpha+\beta)^2(y-x) \\ \\ \dfrac{\big(\underline{a}(\theta)(x-\beta)(x-\alpha)+2\alpha\beta(x-\underline{a}(\theta))\big)(y-\alpha)(\beta-y)}{(y-(\alpha+\beta))(\underline{a}(\theta)(y-(\alpha+\beta))+2\alpha\beta)} \quad \text{otherwise.} \end{cases} \tag{5.13}$$

The maximum in (5.11) is reached for

$$\underline{a}(\theta_h) = \begin{cases} \dfrac{\underline{a}(\theta)}{2}\Big(1+\sqrt{\dfrac{2x-\underline{a}(\theta)}{2y-\underline{a}(\theta)}}\Big) \\ \\ \dfrac{\alpha\beta\underline{a}(\theta)}{\underline{a}(\theta)(y-(\alpha+\beta))+2\alpha\beta} \end{cases} \tag{5.14}$$

in the two cases respectively.

Proposition 5.1 (outer bound) *Let* $A = \begin{pmatrix} x & z \\ z & y \end{pmatrix} \in \mathcal{H}(\theta)$ *then we have*

$$z^2 \le f_\theta(x,y) := \min\{f_a(x,y), f_h(x,y)\}. \tag{5.15}$$

Proof. The proof follows immediately from the estimates above and from (5.4), since

$$\begin{aligned} & \max_{\theta_h,\theta_v} \min\{(\overline{a}(\theta_h)-x)(\overline{a}(\theta_v)-y), (x-\underline{a}(\theta_h))(y-\underline{a}(\theta_v))\} \\ \le\ & \min\{\max_{\theta_h,\theta_v}\{(\overline{a}(\theta_h)-x)(\overline{a}(\theta_v)-y)\}, \max_{\theta_h,\theta_v}\{(x-\underline{a}(\theta_h))(y-\underline{a}(\theta_v))\}\} \\ =\ & \min\{f_a(x,y), f_h(x,y)\}. \end{aligned} \tag{5.16}$$

In the case where $\theta = 1/2$, it is easily deduced from the previous analysis that the expression for $f_{1/2}(x,y)$ in (5.15) is simply given by

$$f_{1/2}(x,y) = \begin{cases} \Big(\dfrac{\alpha+\beta}{2} - \dfrac{x+y}{2}\Big)^2 \text{ if } xy \ge \alpha\beta \\ \\ \left(\dfrac{\alpha\beta}{\alpha+\beta} - \sqrt{\Big(x-\dfrac{\alpha\beta}{\alpha+\beta}\Big)\Big(y-\dfrac{\alpha\beta}{\alpha+\beta}\Big)}\right)^2 \text{ otherwise.} \end{cases}$$

6 Exact bounds for non-diagonal matrices (the case $\theta = 1/2$)

We prove that in the case $\theta = 1/2$ the outer bound given by Proposition 5.1 is optimal.

Theorem 6.1 (exact bounds) *The set* $\mathcal{H}(1/2)$ *is given by all matrices* $A = \begin{pmatrix} x & z \\ z & y \end{pmatrix}$ *such that*

$$\alpha \le x, y \le \beta, \qquad x+y \le \alpha+\beta, \qquad \frac{1}{y}+\frac{1}{x} \le \frac{1}{\alpha}+\frac{1}{\beta},$$

$$z^2 \le \min\left\{\Big(\frac{\alpha+\beta}{2}-\frac{x+y}{2}\Big)^2, \left(\frac{\alpha\beta}{\alpha+\beta} - \sqrt{\Big(x-\frac{\alpha\beta}{\alpha+\beta}\Big)\Big(y-\frac{\alpha\beta}{\alpha+\beta}\Big)}\right)^2\right\}.$$

Proof. Since, because of the equi–boundedness of the approximating sequences, Γ-convergence in the current setting is associated to a metrizable topology (see [3]), $\mathcal{H}(1/2)$ is closed under Γ-convergence. The proof will be achieved by layering on the continuum level. We first note that any solution (x,y,z) to the system $\begin{cases} z^2 = f_a(x,y) \\ z^2 = f_h(x,y) \end{cases}$ lives on the surface of equal determinant $xy - z^2 = \alpha\beta$; hence, we can divide the proof for A satisfying $xy - z^2 \ge \alpha\beta$ and $xy - z^2 \le \alpha\beta$ for which the bounds for the off-diagonal term simply become $z^2 \le f_a(x,y)$ and $z^2 \le f_h(x,y)$, respectively.

The strategy is the following: given A compute the diagonal matrices A_1 and A_2 on the boundary of $\mathcal{H}_d(1/2)$ such that $\det A_i = \det A$; find η and ν such that if we layer A_1 and A_2 with volume fractions η and $(1-\eta)$ in the direction ν we obtain A.

We first perform the proof for $\det A \geq \alpha\beta$ and check the bound $z^2 = f_a(x,y)$. The matrices $A_1 = \begin{pmatrix} s & 0 \\ 0 & t \end{pmatrix}$ and $A_2 = \begin{pmatrix} t & 0 \\ 0 & s \end{pmatrix}$ are characterized by the equations

$$st = xy - z^2 = xy - \Big(\frac{\alpha+\beta}{2} - \frac{x+y}{2}\Big)^2, \tag{6.1}$$

obtained by imposing the 'extremality condition' $z^2 = f_a(x,y)$ to the determinant constraint, and

$$s + t = \alpha + \beta, \tag{6.2}$$

given by the requirement that A_i belong to the boundary of $\mathcal{H}_d(1/2)$.

We layer A_1 and A_2 in proportions $\eta, 1-\eta$ in direction $\nu = (C, S)$ and apply the layering formula in [11] (cf. Proposition 3). The resulting conductivity matrix X is given by

$$(X - A_1)^{-1} = \frac{1}{1-\eta}\Big((A_2 - A_1)^{-1} + \eta\frac{\nu\otimes\nu}{\langle A_1\nu,\nu\rangle}\Big),$$

that is

$$X = \begin{pmatrix} \frac{stC^2+(\eta s+(1-\eta)t)^2S^2}{(\eta C^2+(1-\eta)S^2)t+(\eta S^2+(1-\eta)C^2)s} & -\frac{\eta(1-\eta)(t-s)^2CS}{(\eta C^2+(1-\eta)S^2)t+(\eta S^2+(1-\eta)C^2)s} \\ -\frac{\eta(1-\eta)(t-s)^2CS}{(\eta C^2+(1-\eta)S^2)t+(\eta S^2+(1-\eta)C^2)s} & \frac{stS^2+(\eta s+(1-\eta)t)^2C^2}{(\eta C^2+(1-\eta)S^2)t+(\eta S^2+(1-\eta)C^2)s} \end{pmatrix}.$$

Since $\det A_1 = \det A_2$, Theorem 4 in [5] implies that $\det X = st$. This could also be checked directly with the expression above for X. It thus suffices to prove that we can find η, ν such that

$$\begin{cases} \dfrac{stC^2+(\eta s+(1-\eta)t)^2S^2}{(\eta C^2+(1-\eta)S^2)t+(\eta S^2+(1-\eta)C^2)s} = x \\[2ex] \dfrac{stS^2+(\eta s+(1-\eta)t)^2C^2}{(\eta C^2+(1-\eta)S^2)t+(\eta S^2+(1-\eta)C^2)s} = y \end{cases}$$

as z will thus automatically satisfy $z^2 = st - xy = f_a(x,y)$. This gives a homogeneous system in C^2 and S^2, whose determinant must be zero; i.e.,

$$\begin{aligned} & (st - x(s+\eta(t-s)))(st - y(t-\eta(t-s))) \\ = \; & (t-\eta(t-s))(s+\eta(t-s))(t-\eta(t-s)-x)(s+\eta(t-s)-y). \end{aligned} \tag{6.3}$$

The proportion η is determined by requiring that the volume fractions related to A_1 and A_2 in proportions η and $1-\eta$ must give the volume fractions θ_h, θ_v of A, determined by (5.10). This gives

$$\eta(\beta - s) + (1-\eta)(\beta - t) = \frac{1}{2}\Big((\beta-\alpha) + (y-x)\Big). \tag{6.4}$$

By using (6.1), (6.2) and (6.4), we can easily verify (6.3).

The case $\det A \leq \alpha\beta$ can be proven likewise. In this case, the equal determinant condition (6.1) must be modified by substituting f_a with f_h, thus obtaining

$$st = xy - \left(\frac{\alpha\beta}{\alpha+\beta} - \sqrt{\Big(x - \frac{\alpha\beta}{\alpha+\beta}\Big)\Big(y - \frac{\alpha\beta}{\alpha+\beta}\Big)}\right)^2, \tag{6.5}$$

while (6.2) becomes

$$\frac{1}{s}+\frac{1}{t}=\frac{\alpha+\beta}{\alpha\beta}. \tag{6.6}$$

The proportion η is now determined by (5.14), which gives

$$\eta\frac{\alpha}{s}(\beta-s)+(1-\eta)\frac{\beta}{t}(\beta-t)=\frac{\beta\sqrt{(\alpha+\beta)y-\alpha\beta}-\alpha\sqrt{(\alpha+\beta)x-\alpha\beta}}{\sqrt{(\alpha+\beta)y-\alpha\beta}+\sqrt{(\alpha+\beta)x-\alpha\beta}}. \tag{6.7}$$

By using (6.5)–(6.7), we can again verify (6.3).

7 Concluding remarks

The complete characterization of the set $\mathcal{H}(\theta)$ is missing at present. We conjecture that the outer bound, described in Section 5 (see Proposition 5.1) and found to be optimal in the case $\theta = 1/2$ (see Section 6 above), is optimal for all θ's. As a first result in that direction, we briefly detail how to obtain the optimality of the outer bound for the 'midmatrix' with diagonal elements both equal to $\frac{1}{2}(\overline{a}(\theta)+\underline{a}(\theta))$. The corresponding outer bound yields $z=\pm\frac{1}{2}(\overline{a}(\theta)-\underline{a}(\theta))$, so that the two 'midmatrices' are

$$A_\pm=\begin{pmatrix} \frac{1}{2}(\overline{a}(\theta)+\underline{a}(\theta)) & \pm\frac{1}{2}(\overline{a}(\theta)-\underline{a}(\theta)) \\ \pm\frac{1}{2}(\overline{a}(\theta)-\underline{a}(\theta)) & \frac{1}{2}(\overline{a}(\theta)+\underline{a}(\theta)) \end{pmatrix}.$$

Note that the eigenvalues of $A_\pm$ are $\underline{a}(\theta),\overline{a}(\theta)$ and the eigendirections $\pm\frac{\pi}{4}$.

The construction consists in layering the corresponding outer 'midmatrix' for $\theta = 1/2$, that is

$$B=\begin{pmatrix} \frac{1}{2}(\frac{\alpha+\beta}{2}+\frac{2\alpha\beta}{\alpha+\beta}) & \frac{1}{2}(\frac{\alpha+\beta}{2}-\frac{2\alpha\beta}{\alpha+\beta}) \\ \frac{1}{2}(\frac{\alpha+\beta}{2}-\frac{2\alpha\beta}{\alpha+\beta}) & \frac{1}{2}(\frac{\alpha+\beta}{2}+\frac{2\alpha\beta}{\alpha+\beta}) \end{pmatrix},$$

with αI (resp. βI) in the direction $\frac{\pi}{4}$ and with a volume fraction η such that $\eta\frac{1}{2}+(1-\eta)=\theta$ (resp. $\eta\frac{1}{2}=\theta$). We skip the actual derivation.

Actually, as can be immediately checked by setting $x = y$ in Proposition 5.1, the outer matrices in $\mathcal{H}(\theta)$ such that $x = y$ have an off–diagonal element that grows linearly in x. Since layering $A_\pm$ with the diagonal matrices $\underline{a}(\theta)I$ and $\overline{a}(\theta)I$ — extreme elements of $\mathcal{H}(\theta)$ in the plane $x = y$ of equal diagonal elements — in both directions $\pm\frac{\pi}{4}$ also yields a matrix with an off–diagonal element that grows linearly in $x = y$, we have also established the optimality of the outer bound for all matrices with equal diagonal elements. The computation for general outer matrices in $\mathcal{H}(\theta)$, $\theta\neq\frac{1}{2}$, with distinct diagonal elements remains open at this time.

In a different direction, note that the computations in this study are performed in a fixed basis of the plane. If we allowed the mixture to pick, at each macroscopic point, an optimal orientation of the underlying lattice, thereby generating the equivalent of a polycrystal, the resulting set would certainly be larger than $\bigcap_{U\in SO(2)}(U^t\mathcal{H}(\theta)U)$. But that set will always include diagonal matrices of the form $\underline{a}(\theta)I$ and $\overline{a}(\theta)I$, which cannot be attained at the continuous level by mixing αI with βI in the same volume fraction.

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