Understanding Hashin-Shtrikman Microstructures via Bloch Waves

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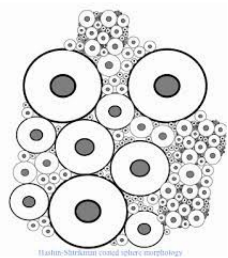
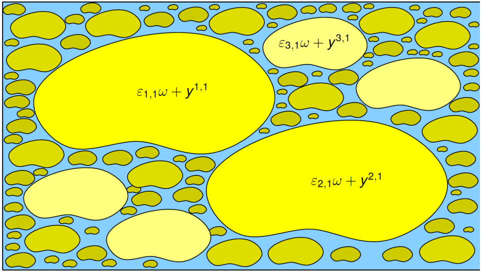
Lecture dedicated to Enrike in the year of his 60^{th} anniversary





Generalized Hashin-Shtrikman (H-S) microstructures

A mathematical construction in the context of heat conducting materials/media

The construction/definition of an H-S microstructure in an open region $\Omega \subseteq \mathbb{R}^N$ involves two basic ingredients of homogenization theory:

1. The notion of G-convergence or H-convergence
2. A geometric configuration
   A sequence of conductive materials whose heterogeneities obey certain (geometrical) rules of composition / distribution

H-convergence

- A heat conducting material in Ω is represented by its conductivity tensor, say $A = A(x) = [a_{k\ell}(x)], x \in \Omega$.
- The coefficients $a_{k\ell}$ are assumed to be measurable, bounded, and satisfying a uniform ellipticity condition in Ω.

$$(A^\varepsilon)_{\varepsilon\to 0} \xrightarrow{\text{H}} A^*$$

$$\Updownarrow$$

For all $f \in H^{-1}(\Omega)$, the sequence of solutions $u^\varepsilon \in H_0^1(\Omega)$ of

$$-\mathrm{div}\,(A^\varepsilon(x)\nabla u^\varepsilon) = f \quad \text{in} \quad \Omega, \qquad \text{satisfies}$$

1. $u^\varepsilon \rightharpoonup u^* \quad \text{in} \quad H_0^1(\Omega)$-weakly
2. $A^\varepsilon \nabla u^\varepsilon \rightharpoonup A^* \nabla u^* \quad \text{in} \quad L^2(\Omega)$-weakly,

where u^* is the solution of

$$-\mathrm{div}\,(A^*(x)\nabla u^*) = f \quad \text{in} \quad \Omega.$$

A classical model situation: Periodic homogenization

with period say $Y = (0, 2\pi)$ in $\mathbb{R}^n$

The sequence of conductivity tensors $(A^\varepsilon)_\varepsilon$ has the generic form

$$A^\varepsilon(x) = A^Y\left(\frac{x}{\varepsilon}\right) \qquad x \in \Omega,$$

where $A^Y = A^Y(y)$ is Y-periodic.

- The H-limit of $(A^\varepsilon)_\varepsilon$, say $A^* = [a^*_{k\ell}]$, is a constant tensor.
- Explicit formulae for the homogenized coefficients are available in terms of the coefficients $[a^Y_{k\ell}(y)]$ of the tensor $A^Y(y)$.

The geometric configuration

behind the Hashin-Shtrikman microstructures

Let $\omega \subset \mathbb{R}^N$ be a bounded open subset with a Lipschitz boundary

- ω will play the role of Y, let us call it the reference motif or reference icon

Definition A sequence (indexed by $n \in \mathbb{N}$) of Vitali's coverings of Ω by reduced and disjoint copies of ω, is a sequence of coverings, say

$$\{\bigcup_{p\in K_n}(\epsilon_{p,n}\omega + y^{p,n})\}_{n\in\mathbb{N}}$$

where K_n is finite or countable, and for any $n \in \mathbb{N}$

- $(\varepsilon_{p,n}\omega + y^{p,n}) \cap (\varepsilon_{q,n}\omega + y^{q,n}) = \emptyset \qquad \forall p, q \in K_n, \quad p \neq q$
- $meas(\Omega \setminus \bigcup_{p\in K_n}(\epsilon_{p,n}\omega + y^{p,n})) = 0$
- If $\kappa_n \overset{(\mathrm{def})}{=} \sup_{p\in K_n} \epsilon_{p,n}$, then $\kappa_n \to 0$ as $n \to \infty$

The geometric configuration, illustrated

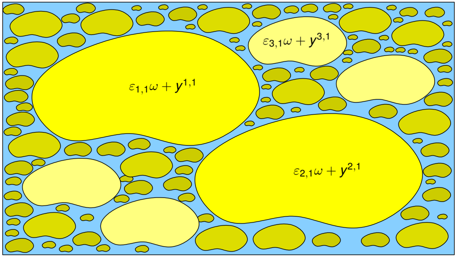
A Vitali's sequence of disjoint coverings of Ω is obtained by moving reduced copies of ω to different positions $y^{p,n}$ inside Ω:

$$meas(\Omega \setminus \bigcup_{p \in K_n} (\varepsilon_{p,n}\,\omega + y^{p,n})) = 0, \qquad \kappa_n \overset{\text{(def)}}{=} \sup_{p \in K_n} \varepsilon_{p,n} \to 0,$$

Vitali's sequence

$n = 1$

$\kappa_1 = \sup_{p \in K_1} \varepsilon_{p,1}$



A sequence of conductive materials associated with a sequence of Vitali's coverings of Ω

Let us fill in ω with an arbitrary heterogeneous material with conductivity tensor $A = A^{\omega}(y) = [a^{\omega}_{k\ell}(y)]$

Next, we fill in Ω by mixing this material $A^{\omega}(y)$ according to the geometric configuration defined by a sequence of Vitali's coverings.

Precesily, for each $n \in \mathbb{N}$ and for a.e. $x \in \Omega$, $\exists!\ p \in K_n$ (depending on x) s.t. $x \in (\epsilon_{p,n}\omega + y^{p,n})$ and $\frac{x-y^{p,n}}{\epsilon_{p,n}} \in \omega$. Define

$$A^{n,\omega}(x) = A^{\omega}\left(\frac{x - y^{p,n}}{\varepsilon_{p,n}}\right)$$

This represents a Hashin-Shtrikman microstructure in Ω.

H-convergence of a Hashin-Shtrikman microstructure

Definition Given an H-S microstructure $A^{n,\omega}$ with conductivity tensor $A^{\omega}(\cdot)$, let's address the following questions:

- Does $(A^{n,\omega})_n$ is H-convergent?, i.e., is there a limit tensor Q such that

$$A^{n,\omega} \xrightarrow{\text{H}} Q \quad \text{in} \quad \Omega\ ?,$$

- and if it does

$$\text{How } Q \text{ can be get from } A^{\omega}(\cdot)\ ?$$

A first example

A. Hashin & S. Shtrikmann (1962), *J. Appl. Phys.*

Example (Spherical inclusions in two-phase medium)

Let $\omega = B(0,1) = \{y : |y| < 1\}$ and $R \in (0,1)$. We consider the micro-structure

$$A^\omega(y) = \begin{cases} \alpha I & \text{if} \quad |y| \leq R, \\ \beta I & \text{if} \quad R < |y| \leq 1 \end{cases}$$

Then A^ω H-converges to γI, where γ satisfies:

$$\frac{\gamma - \beta}{\gamma + (N-1)\beta} = \theta \frac{\alpha - \beta}{\alpha + (N-1)\beta}, \quad \text{with } \theta = R^N.$$

Bloch waves in H-S microstructures

Spectral problem in ω

$$(SP)\begin{cases} \mathcal{A}^\omega(\eta)\varphi^\omega(y;\eta) = \lambda^\omega(\eta)\varphi^\omega(y;\eta) \quad \text{in} \quad \omega, \\ \varphi^\omega(y;\eta) \text{ is constant on } \partial\omega, \quad \displaystyle\int_{\partial\omega} a^\omega_{k\ell}(y)\Big(\frac{\partial}{\partial y_\ell} + i\eta_\ell\Big)\varphi^\omega(y;\eta)\nu_k \, d\sigma = 0, \end{cases}$$

where

$$\mathcal{A}^\omega(\eta) \overset{\text{(def)}}{=} -\Big(\frac{\partial}{\partial y_k} + i\eta_k\Big)\Big[a^\omega_{k\ell}(y)\Big(\frac{\partial}{\partial y_\ell} + i\eta_l\Big)\Big]$$

Theorem (Existence result) Fix $\eta \in \mathbb{R}^N$. Then $\exists$ a sequence of eigenvalues $\{\lambda^\omega_m(\eta); m \in \mathbb{N}\}$ and corresponding eigenvectors $\{\varphi^\omega_m(y;\eta) \in H^1_c(\omega), m \in \mathbb{N}\}$ of (SP) s.t.

- $0 \leq \lambda^\omega_1(\eta) < \lambda^\omega_2(\eta) \leq \cdots \to \infty$ (each one of finite multiplicity)
- $\{\varphi^\omega_m(\cdot;\eta); \; m \in \mathbb{N}\}$ is an orthonormal basis for $L^2_c(\omega)$

The state spaces are

$$L^2_c(\omega) = \{\varphi \in L^2_{loc}(\mathbb{R}^N) \mid \varphi \text{ is constant in } \mathbb{R}^N \setminus \omega\}$$

$$H^1_c(\omega) = \{\varphi \in H^1_{loc}(\mathbb{R}^N) \mid \varphi \text{ is constant in } \mathbb{R}^N \setminus \omega\}$$

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Regularity of the ground state

Properties

1. There exists a neighborhood around $\eta = 0$ s.t.

$$\eta \longmapsto (\lambda_1^\omega(\eta), \varphi_1^\omega(\cdot;\eta)) \in \mathbb{C} \times H_c^1(\omega) \quad \text{is analytic}$$

2. There is a choice of the first eigenvector $\varphi_1^\omega(y;\eta)$ s.t. $\varphi_1^\omega(y;\eta) = |\omega|^{-1/2} \quad \forall y \in \partial\omega, \forall \eta$ in the neighborhood

Computation of derivatives: $\forall k, \ell$

- $D_k \lambda_1(0) = 0 \quad \forall k = 1, ..., N$
- $\dfrac{1}{2} \dfrac{\partial^2 \lambda_1^\omega}{\partial \eta_k \partial \eta_\ell}(0) = \; q_{kl}$

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An H-S microstructure equivalent to a matrix $Q = [q_{k\ell}]$

Definition An H-S microstructure with conductivity tensor $A^\omega(\cdot)$ is said to be equivalent to a positive definite constant matrix Q if, after extending A^ω by $A^\omega(y) = Q$ for $y \in \mathbb{R}^N \setminus \omega$,

For all $\lambda \in \mathbb{R}^N$ there exists a $w_\lambda \in H^1_{loc}(\mathbb{R}^N)$ satisfying

- $-\mathrm{div}_y\big(A^\omega(y)\nabla_y w_\lambda(y)\big) = 0 \quad \text{in} \quad \mathbb{R}^N$
- $w_\lambda(y) = \lambda \cdot y \quad \text{in} \quad \mathbb{R}^N \setminus \omega$

The function w_λ can be equivalently obtained solving the following problem in ω:

- $-\mathrm{div}_y\big(A^\omega(y)\nabla_y w_\lambda(y)\big) = 0 \quad \text{in} \quad \omega$
- $w_\lambda(y) - \lambda \cdot y \in H^1_0(\omega)$

  with the additional boundary condition

- $A_\omega \nabla w_\lambda \cdot \nu = Q\lambda \cdot \nu$ on $\partial\omega$

First main result in Hashin-Shtrikman

Homogenization result in H-S

Theorem Let $A^{\omega,n}$, $Q = [q_{k,\ell}]$ be defined as before. Assume that $A^{\omega}(\cdot)$ is equivalent to Q. Let $f \in L^2(\Omega)$ and consider $u^n \in H_0^1(\Omega)$ be the unique solution of

$$-\mathrm{div}\left(A^{\omega,n}(x)\nabla u^n\right) = f \quad \text{in} \quad \Omega.$$

Then there exists $u \in H_0^1(\Omega)$ s.t.

- $u^n \rightharpoonup u^* \quad$ weakly in $H_0^1(\Omega)$
- $A^{\omega,n}\nabla u^n \rightharpoonup Q\nabla u^* \quad$ weakly in $L^2(\Omega)^N$.

In particular, the limit u^* satisfies (the homogenized equation)

$$-\mathrm{div}\left(Q\nabla u^*\right) = -\sum_{k,\ell} \frac{\partial}{\partial x_k}\left(q_{k\ell}\frac{\partial u^*}{\partial x_\ell}\right) = f \quad \text{in} \quad \Omega$$

Happy Birthday Enrike