



The Dispersion Tensor and Its Unique Minimizer in Hashin–Shtrikman Micro-structures

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Abstract

In this paper, we introduce a macroscopic quantity, namely the dispersion tensor or the *Burnett coefficients* in the class of generalized Hashin–Shtrikman micro-structures (Tartar in *The general theory of homogenization*, volume 7 of Lecture notes of the Unione Matematica Italiana, Springer, Berlin, p 281, 2009). In the case of two-phase materials associated with the periodic Hashin–Shtrikman structures, we settle the issue that the dispersion tensor has a unique minimizer, which is the so called Apollonian–Hashin–Shtrikman micro-structure.

1. Introduction

This paper is concerned with a higher order approximation for a class of elliptic equations in heterogeneous media defined by the well-known generalized Hashin–Shtrikman (HS) micro-structures [13, 14, 18], [20, page no. 281]. In these references a first order approximation, known as the homogenized medium, is given, and it has been defined by the homogenized tensor A^* . In this work, we propose to go further and introduce an approximate medium to the next order of accuracy. While the homogenized tensor A^* has indeed been introduced for arbitrary micro-structures, higher order approximation has been introduced and studied mainly for periodic micro-structures [2, 7–10]. See also [3] and [12]. This is made possible because of the spectral approach to the homogenization problem using Bloch waves [11], which naturally leads to other macroscopic quantities apart from A^* . It is important to remark that HS micro-structures need not be periodic. In our previous work [4], we extended the spectral approach and introduced Bloch waves in HS micro-structures. We also gave a spectral interpretation of the homogenized tensor A^* associated with HS micro-structures. Our goal here is to use the same Bloch waves and consider the higher-order tensor d , called the dispersion tensor in [4], and study some of its properties.

Periodic micro-structures enjoy an invariance property with respect to translation and dilation and Bloch wave construction on such micro-structures can be based on it. Looking at the construction of HS micro-structures, this simple invariance property is lost and this is the origin of the difficulties. It is an open problem to introduce Bloch waves for general non-periodic micro-structures.

Below we make several points comparing the tensors A^* and d on general periodic micro-structures and on HS micro-structures. We mainly (though not exclusively) focus on such micro-structures with two phases α, β in a given proportion θ . First of all, d is a tensor whose order is higher than that of A^* . In the model considered here, A^* is a second order tensor whereas d is a fourth order tensor. In the one-dimensional case, however, both are scalar quantities. It is well-known that in one dimension, the value of A^* coincides with the harmonic mean of the two-phases with the given proportion. Thus, A^* is fixed once these three macro quantities associated with the micro-structure are given. In comparison, d depends on finer scale features of the periodic micro-structure apart from these three quantities and consequently, it shows variation. The extent of its variation on periodic micro-structures keeping these macro quantities fixed is described in our earlier work [9, 10], and is seen by obtaining optimal bounds independent of micro-structures in one-dimension and multi-dimensional laminates. Similar properties of d hold true among HS micro-structures too.

In terms of acoustic waves propagating in periodic micro-structures, the eigenvalues of the matrix A^* represent approximate overall speeds in directions defined by eigenvectors common to all wavelengths, whereas d describes the changes in speeds due to the dispersion of waves, depending on their wavelengths. More precisely, for each wave number defined by a vector η , the eigenvalues of the matrix $d \eta \cdot \eta$ represent changes due to dispersion in the speeds of waves corresponding to the wave number η . Necessarily, A^* is a scale independent quantity whereas d is scale dependent.

A more refined property of d was established in [7], namely, that d has a sign irrespective of the underlying periodic micro-structure and it is non-positive; in contrast, it is well-known that A^* has a sign which is positive for arbitrary micro-structures. It is generally accepted that higher order macro quantities do not possess a sign and that is why it was a bit surprising that d has a sign.

Let us now motivate the optimal bounds on macro quantities independent of micro-structures. Consider the general optimal design problem (ODP) of micro-structures with (isotropic) two-phases in a given proportion to design a good conductor (or) an insulator. This is a well-studied problem [2] in which the state equation is defined by a div-form elliptic operator with scalar coefficients taking two phase values. The result is that there is, in general, no solution among two-phase media, which we refer to as classical micro-structure; however, there are solutions among mixtures of such micro-structures represented by homogenized tensors A^* . The celebrated result of Murat–Tartar [17, 19] characterizes all such tensors A^* via optimal bounds on their eigenvalues. In Figure 1, the region defined by these bounds is depicted. It is a convex lens shaped region which is shaded. Some distinguished extremal points A, B, M, N are marked. The points A, B correspond to

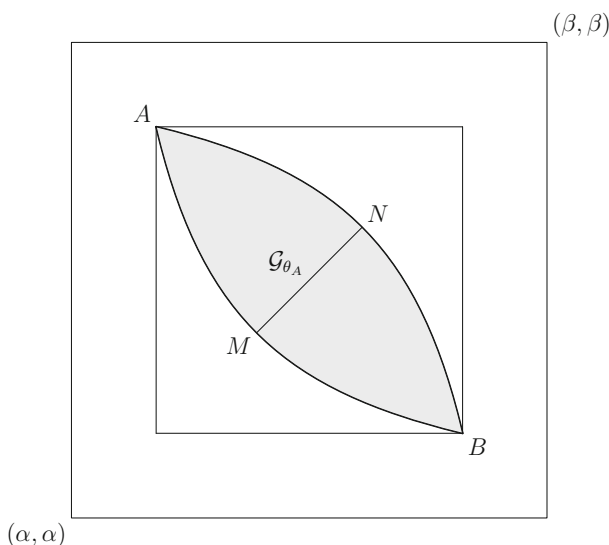


Fig. 1. Murat–Tartar Bounds.

mixtures of simply laminated micro-structures and the points M , N correspond to HS micro-structures.

Next, let us consider ODP in which we replace the previous elliptic equation by the associated wave equation. As before, to obtain a solution to this ODP within a suitable class of mixtures, we need to approximate the state equation. A first such approximation is given by the homogenized wave equation. However this does not take into account dispersive effects caused by the micro-structure. An improved approximate model including dispersion has been derived [2], [12] in the case of periodic micro-structures. These models are relevant if we wish to optimize dispersion by adjusting micro-structures; for instance, we may desire to minimize dispersion as in fibre optics cables. The model obtained in [2] is given by an equation which contains both macro quantities A^* , d . As in the elliptic case, with a motivation to describe all such approximations, we seek optimal bounds on d , since bounds for A^* are already known from [17]. This is a long term goal regarding this subject. There are a few such rigorous bounds on d in the literature [9, 10]. The works mentioned are motivated by the desire to see the extent of variation of d on the extremal structures for A^* . Accordingly, this programme was carried out for laminated micro-structures which correspond to the points A , B in the Figure 1. In this paper, we continue this task and deal with the points M , N which represent HS micro-structures. This is not a trivial job because, as remarked earlier, unlike A^* , the tensor d uses some small scale features of micro-structures. For numerical implementation of ODP for dispersion, see [3].

Various points in the phase diagram for A^* (Figure 1) are obtained by homogenizing two-phase micro-structures and hence they represent conductivities of the mixture of two-phases in given proportion. This is the reason why there are no solutions to ODP among classical two-phase micro-structures. Strangely, this is not

the case for certain ODP for dispersion; it admits two-phase micro-structures as optimizers. Furthermore, such optimizers are unique. This is yet another property which distinguishes d from A^* . In general, micro-structures underlying a point in the phase diagram for A^* are not unique. For instance, the point M in Figure 1 is obtained by homogenizing arbitrary HS micro-structures as long as they possess the same macro parameters α , β , θ and there are plenty of them. The above unique property of d was first noticed in the study [9] of one dimensional case. Roughly speaking, it was noted that d increases as we increase the number of interfaces between the two-phases in the micro-structure. At the minimum value therefore, the micro-structure is unique and it is defined by two intervals on which the two phase values are taken. It is therefore natural to seek a multi-dimensional analogue of the above result. Our insight into the structure of d and some numerical experiments with HS micro-structures suggested a *conjecture* for a possible candidate for the minimizer among periodic HS micro-structures and we call it the Apollonian–Hashin–Shtrikman micro-structure. This article is devoted to the preparation and the resolution of this *conjecture*.

More precisely, we prove that d has a unique minimizer (called Apollonian–Hashin–Shtrikman micro-structure); by its very geometrical construction, it has minimal number of balls compared to an arbitrary Hashin–Shtrikman micro-structure: each time a ball is inserted in the medium in such a way that it occupies maximum available volume and hence it contains minimum number of balls. These balls act as scatterers for the waves propagating in the medium obeying laws of refraction at the interfaces and thus they are responsible for the dispersion of waves. It is common sense that fewer scatterers imply less dispersion. This intuitive feeling is confirmed by our result, namely: minimum dispersion is produced by a Apollonian–Hashin–Shtrikman micro-structure.

Some easy consequences of our result are mentioned below. Though d depends on finer scale features on the micro-structure, it was found [9, 10] that the optimal bounds depend only on the three macro quantities α , β , θ . Our previous study also indicated the dependence of d on the measure of interface between the two-phases in the micro-structure, apart from the three macro quantities. However, this dependence is not very explicit even at the minimum value of d as shown by Apollonian–Hashin–Shtrikman micro-structure. In contrast, the optimal bounds for A^* are quite explicit involving the three parameters, as shown by Murat–Tartar Theorem [17].

Usually, ODP do not admit solutions among classical micro-structures. It will be a rare exceptional situation if such solutions are found. That is why relaxed micro-structures (also known as mixtures (or) homogenized structures) are introduced and solutions are found among them. Once a relaxed micro-structure is found as a solution to ODP, the usual practice is to suggest a penalized micro-structure which is a classical micro-structure and which is an approximation to the relaxed micro-structure with respect to H-topology (see [1]). A minimum dispersion problem among HS micro-structures is one of those exceptional situations which admits classical micro-structure as a solution and there is no need for penalization.

Let us end this Introduction by presenting a plan of the organization of this paper. After this Introduction, we devote two sections (Section 2 and Section 3)

to recall elements of Bloch wave analysis on general periodic micro-structures, and then on generalized Hashin–Shtrikmann (HS) micro-structures with arbitrary inclusion (which are not necessarily periodic). We also establish their link with the homogenized and dispersion tensors on such structures. This material is borrowed from our work in [4]. In Section 4, we specialize to HS micro-structures with spherical inclusions and impose periodicity on them. Homogenized and dispersion tensors reduce to scalars in this case. Finally, in Section 5, we solve the problem of minimizing the dispersion coefficient on periodic HS micro-structures (with spherical inclusions) and show that there is a unique minimizer and that is Apollonian–Hashin–Shtrikman micro-structure which is also defined in this section.

2. Preliminaries

In the beginning, we remark that the summation with respect to the repeated indices is understood throughout this paper. Let us start with the known periodic case.

2.1. Dispersion Tensor and Periodic Structures

We consider the operator

$$A_Y \equiv -\frac{\partial}{\partial y_k} \left(a_{kl}^Y(y) \frac{\partial}{\partial y_l} \right), \quad y \in \mathbb{R}^N,$$

where the coefficient matrix $A_Y(y) = [a_{kl}^Y(y)]$ defined on Y almost everywhere with $Y = [0, 1]^N$ is known as the periodic cell and $A_Y \in \mathcal{M}(\alpha, \beta; Y)$ for some $0 < \alpha < \beta$, that is

$$a_{kl}^Y = a_{lk}^Y \quad \forall k, l \text{ and } (A_Y(y)\xi, \xi) \geq \alpha|\xi|^2, \quad |A_Y(y)\xi| \leq \beta|\xi| \text{ for any } \xi \in \mathbb{R}^N, \\ \text{almost everywhere on } Y.$$

For each $\varepsilon > 0$, we consider the ε -periodic elliptic operator

$$\mathcal{A}_Y^\varepsilon \equiv -\frac{\partial}{\partial x_k} \left(a_{kl}^Y\left(\frac{x}{\varepsilon}\right) \frac{\partial}{\partial x_l} \right), \quad x \in \mathbb{R}^N,$$

where x (slow variable) and y (fast variable) are related by $y = \frac{x}{\varepsilon}$. We now define the Bloch waves ψ_Y associated with the operator \mathcal{A}_Y . Let us consider the following spectral problem parametrized by $\eta \in \mathbb{R}^N$: find $\lambda_Y = \lambda_Y(\eta) \in \mathbb{R}$ and $\psi_Y = \psi_Y(y; \eta)$ (not zero) such that

$$A_Y \psi_Y(\cdot; \eta) = \lambda_Y(\eta) \psi_Y(\cdot; \eta) \quad \text{in } \mathbb{R}^N, \quad \psi_Y(\cdot; \eta) \text{ is } (\eta; Y)\text{-periodic, that is} \\ \psi_Y(y + 2\pi m; \eta) = e^{2\pi i m \cdot \eta} \psi_Y(y; \eta) \quad \forall m \in \mathbb{Z}^N, \quad y \in \mathbb{R}^N.$$

Next, by Floquet theory, we define $\varphi_Y(y; \eta) = e^{iy \cdot \eta} \psi_Y(y; \eta)$ to rewrite the above spectral problem as follows:

$$\mathcal{A}_Y(\eta)\varphi_Y = \lambda_Y(\eta)\varphi_Y \quad \text{in } \mathbb{R}^N, \quad \varphi_Y \text{ is } Y\text{-periodic.} \tag{2.1}$$

Here the operator $\mathcal{A}_Y(\eta)$ is called the translated operator and is defined by

$$\mathcal{A}_Y(\eta) = e^{-iy \cdot \eta} \mathcal{A}_Y e^{iy \cdot \eta} = -\left(\frac{\partial}{\partial y_k} + i\eta_k\right) \left[a_{kl}^Y(y) \left(\frac{\partial}{\partial y_l} + i\eta_l\right) \right].$$

It is well known that for $\eta \in Y' = [-\frac{1}{2}, \frac{1}{2}]^N$ the dual torus, the above spectral problem (2.1) admits a discrete sequence of eigenvalues and their eigenfunctions referred to as Bloch waves introduced above enable us to describe the spectral resolution of \mathcal{A}_Y an unbounded self-adjoint operator in $L^2(\mathbb{R}^N)$ in the orthogonal basis $\{e^{iy \cdot \eta} \varphi_{Y,m}(y; \eta) | m \geq 1, \eta \in Y'\}$.

To obtain the spectral resolution of $\mathcal{A}_Y^\varepsilon$, we introduce Bloch waves at the ε -scale as

$$\lambda_{Y,m}^\varepsilon(\xi) = \varepsilon^{-2} \lambda_{Y,m}(\eta), \quad \psi_{Y,m}^\varepsilon(x; \xi) = \psi_{Y,m}(y; \eta), \quad \varphi_{Y,m}^\varepsilon(x; \xi) = \varphi_{Y,m}(y; \eta),$$

where the variables (x, ξ) and (y, η) are related by $y = \frac{x}{\varepsilon}$ and $\eta = \varepsilon\xi$. Observe that $\varphi_{Y,m}^\varepsilon(x; \xi)$ is εY -periodic (in x) and $\varepsilon^{-1} Y'$ -periodic with respect to ξ . In the same manner, $\psi_{Y,m}^\varepsilon(\cdot; \xi)$ is $(\varepsilon\xi; \varepsilon Y)$ -periodic. The dual cell at ε -scale, where ξ varies, is $\varepsilon^{-1} Y'$.

We consider a sequence $u^\varepsilon \in H^1(\mathbb{R}^N)$ satisfying

$$\mathcal{A}_Y^\varepsilon u^\varepsilon = f \quad \text{in } \mathbb{R}^N, \tag{2.2}$$

with the fact $u^\varepsilon \rightharpoonup u$ in $H^1(\mathbb{R}^N)$ weak and $u^\varepsilon \rightarrow u$ in $L^2(\mathbb{R}^N)$ strong.

The homogenization problem consists of passing to the limit in (2.2), as $\varepsilon \rightarrow 0$ and we get the homogenized equation satisfied by u , namely

$$\mathcal{A}_Y^* u = -\frac{\partial}{\partial x_k} \left(q_{kl} \frac{\partial u}{\partial x_l} \right) = f \quad \text{in } \mathbb{R}^N,$$

where $A_Y^* = [q_{kl}]$ is the constant homogenized matrix (see [1]).

Simple relation linking A_Y^* with Bloch waves is the following: $q_{kl} = \frac{1}{2} D_{kl}^2 \lambda_{Y,1}(0)$ (see [5, 11]). At this point, it is appropriate to recall that derivatives of the first eigenvalue and eigenfunction at $\eta = 0$ exist, thanks to the regularity property established in [6, 11].

Proposition 2.1. (Regularity of the ground state [6, 11])

Under the periodic assumption on the matrix $A_Y \in \mathcal{M}(\alpha, \beta; Y)$, there exists $\delta > 0$ such that the first eigenvalue $\lambda_{Y,1}(\eta)$ is an analytic function on $B_\delta(0) = \{\eta \in \mathbb{R}^N \mid |\eta| < \delta\}$ and there is a choice of the first eigenvector $\varphi_{Y,1}(y; \eta)$ satisfying

$$\eta \mapsto \varphi_{Y,1}(\cdot; \eta) \in H_{\#}^1(Y) \text{ is analytic on } B_\delta \text{ and } \varphi_{Y,1}(y; 0) = |Y|^{-1/2}.$$

Moreover, we have the following relations:

$$\begin{aligned} \lambda_{Y,1}(0) &= 0, \quad D_k \lambda_{Y,1}(0) = \frac{\partial \lambda_{Y,1}}{\partial \eta_k}(0) = 0 \quad \forall k = 1, \dots, N. \\ \varphi_{Y,1}(\cdot, 0) &= |Y|^{-1/2}, \quad D_k \varphi_{Y,1}(\cdot, 0) = i|Y|^{-1/2} \chi_k(y), \\ \frac{1}{2} D_{kl}^2 \lambda_{Y,1}(0) &= \frac{1}{2} \frac{\partial^2 \lambda_{Y,1}}{\partial \eta_k \partial \eta_l}(0) = q_{kl} \quad \forall k, l = 1, \dots, N, \end{aligned}$$

where the last expression is considered as the Bloch spectral representation of the homogenized tensor, which are essentially defined as

$$\frac{1}{2} D_{kl}^2 \lambda_{Y,1}(0) = q_{kl} = \frac{1}{|Y|} \int_Y A_Y (\nabla \chi_k + e_k) \cdot (\nabla \chi_l + e_l) dy \quad (2.3)$$

for each unit vector e_k and the functions $\chi_k \in H_{\#}^1(Y)$ solving the following conductivity problem in the periodic unit cell:

$$-\operatorname{div}_y (A_Y(y) (\nabla_y \chi_k(y) + e_k)) = 0 \quad \text{in } Y, \quad y \mapsto \chi_k(y) \text{ is } Y\text{-periodic.}$$

Moreover, all odd order derivatives of $\lambda_{Y,1}$ at $\eta = 0$ are zero, that is

$$D^q \lambda_{Y,1}(0) = 0 \quad \forall q \in \mathbb{Z}_+^N, |q| \text{ odd.}$$

Additionally, all even order derivatives need to not be zero and can be calculated in a systematic way.

The fourth order derivative of $\lambda_{Y,1}$ at $\eta = 0$ is non-zero and known as the **Burnett coefficient** or the **dispersion tensor** d_Y of the medium,

$$\frac{1}{4!} \frac{\partial^4 \lambda_{Y,1}(0)}{\partial \eta_k \partial \eta_l \partial \eta_m \partial \eta_n} \eta_k \eta_l \eta_m \eta_n = d_{klmn} \eta_k \eta_l \eta_m \eta_n = d_Y \eta^4, \quad (2.4)$$

which is essentially a non-positive definite fourth order tensor and can be expressed as follows: let us call $D_{kl}^2 \varphi_{Y,1}(\cdot; 0) = |Y|^{-1/2} \chi_{kl}$ and define

$$\begin{aligned} C_Y &= \eta_n C_n^Y \quad \text{with} \quad C_n^Y(\varphi) = -a_{nj}^Y(y) \frac{\partial \varphi}{\partial y_j} - \frac{\partial}{\partial y_j} (a_{nj}^Y(y) \varphi), \\ X_Y^{(1)} &= \eta_n \chi_n, \quad X_Y^{(2)} = \eta_k \eta_n \chi_{kn}, \quad \widetilde{A}_Y = \eta_k \eta_n a_{kn}^Y, \quad \widetilde{A}_Y^* = \eta_k \eta_n q_{kn}, \end{aligned} \quad (2.5)$$

satisfying

$$-\operatorname{div} (A_Y \nabla X_Y^{(1)}) = \eta_k \frac{\partial a_{kl}^Y}{\partial y_l} \text{ in } Y, \quad X_Y^{(1)} \in H_{\#}^1(Y) \text{ with } \int_Y X_Y^{(1)} dy = 0$$

and

$$-\operatorname{div} (A_Y \nabla X_Y^{(2)}) = (\widetilde{A}_Y - \widetilde{A}_Y^*) - C_Y X_Y^{(1)} \text{ in } Y, \quad X_Y^{(2)} \in H_{\#}^1(Y) \text{ with } \int_Y X_Y^{(2)} dy = 0. \quad (2.6)$$

Then, by summation, one has the following expression of the dispersion tensor:

$$d_Y \eta^4 = -\frac{1}{|Y|} \int_Y A_Y \left(X_Y^{(2)} - \frac{(X_Y^{(1)})^2}{2} \right) \cdot \left(X_Y^{(2)} - \frac{(X_Y^{(1)})^2}{2} \right) \leq 0. \quad (2.7)$$

Remark 2.1. In order to see the role of the dispersion tensor d_Y that arises in wave propagation problems, let us consider the wave propagation problem in periodic structure governed by the operator $\partial_{tt} + \mathcal{A}_Y^\varepsilon$ with appropriate initial conditions. As we see, we have

$$\begin{aligned} \lambda_{Y,1}^\varepsilon(\xi) &\approx \frac{1}{2!} \lambda_{Y,1}^{(2)}(0) \xi^2 \quad \text{if } \varepsilon^2 |\xi|^4 \text{ is small,} \\ \lambda_{Y,1}^\varepsilon(\xi) &\approx \frac{1}{2!} \lambda_{Y,1}^{(2)}(0) \xi^2 + \frac{1}{4!} \varepsilon^2 \lambda_{Y,1}^{(4)}(0) \xi^4 \quad \text{if } \varepsilon^4 |\xi|^6 \text{ is small.} \end{aligned}$$

Thus, if we consider short waves of low energy with wave number satisfying $\varepsilon^2 |\xi|^4 = \mathcal{O}(1)$ and $\varepsilon^4 |\xi|^6 = o(1)$, then a simplified description is obtained with the operator $\partial_{tt} + \mathcal{A}_Y^* + \varepsilon^2 D_Y$, where D_Y is the fourth-order operator whose symbol is $\frac{1}{4!} \frac{\partial^4 \lambda_{Y,1}(0)}{\partial \eta_k \partial \eta_l \partial \eta_m \partial \eta_n} \xi_k \xi_l \xi_m \xi_n$.

2.2. *Survey of Bloch waves, Bloch eigenvalues and eigenvectors in Hashin–Shtrikman structure*

In this part, we recall our recent work [4] of introducing Bloch waves and associated Bloch spectral analysis in the class of generalized Hashin–Shtrikman micro-structures concerning the homogenization result.

Hashin–Shtrikman micro-structures

We follow [20, page no. 281] in this sequel. Let $\omega \subset \mathbb{R}^N$ be a bounded open subset with Lipschitz boundary. Let $A_\omega(y) = [a_{kl}^\omega(y)]_{1 \leq k, l \leq N} \in \mathcal{M}(\alpha, \beta; \omega)$ be such that after extending A_ω by $A_\omega(y) = M$ for $x \in \mathbb{R}^N \setminus \omega$, where $M \in L_+(\mathbb{R}^N; \mathbb{R}^N)$ (that is $M = [m_{kl}]_{1 \leq k, l \leq N}$ is a constant positive definite $N \times N$ matrix), if for each $\lambda \in \mathbb{R}^N$ there exists $w_\lambda \in H_{loc}^1(\mathbb{R}^N)$ satisfying

$$-\operatorname{div}(A_\omega(y) \nabla w_\lambda(y)) = 0 \quad \text{in } \mathbb{R}^N, \quad w_\lambda(y) = (\lambda, y) \quad \text{in } \mathbb{R}^N \setminus \omega, \quad (2.8)$$

then A is said to be *equivalent* to M .

Then one uses a sequence of Vitali coverings of Ω by reduced copies of ω :

$$\operatorname{meas}\left(\Omega \setminus \bigcup_{p \in K} (\varepsilon_{p,n} \omega + y^{p,n})\right) = 0, \quad \text{with } \kappa_n = \sup_{p \in K} \varepsilon_{p,n} \rightarrow 0, \quad (2.9)$$

for a finite or countable K . These define the micro-structures in A_ω^n . One defines, for almost everywhere $x \in \Omega$,

$$A_\omega^n(x) = A_\omega\left(\frac{x - y^{p,n}}{\varepsilon_{p,n}}\right) \quad \text{in } (\varepsilon_{p,n} \omega + y^{p,n}), \quad p \in K, \quad (2.10)$$

which makes sense since, for each n , the sets $(\varepsilon_{p,n} \omega + y^{p,n})$, $p \in K$ are disjoint. The above construction (2.10) represents the so called **Hashin–Shtrikman** micro-structures.

Following that, one defines $v^n \in H^1(\Omega)$ by

$$v^n(x) = \varepsilon_{p,n} w_\lambda \left(\frac{x - y^{p,n}}{\varepsilon_{p,n}} \right) + (\lambda, y^{p,n}) \quad \text{in } (\varepsilon_{p,n} \omega + y^{p,n}). \quad (2.11)$$

Then one has the following properties (see [20, Page no. 283]):

$$\begin{aligned} v^n(x) &\rightharpoonup (\lambda, x) \text{ weakly in } H^1(\Omega; \mathbb{R}^N), \\ A_\omega^n \nabla v^n(x) &\rightharpoonup M\lambda \text{ weakly in } L^2(\Omega; \mathbb{R}^N), \\ -\operatorname{div}(A_\omega^n(x) \nabla v^n(x)) &= 0 \text{ in } \Omega. \end{aligned} \quad (2.12)$$

Thus, by the definition of H -convergence (see [20, Page no. 82]), one has the following convergence of the entire sequence:

$$A_\omega^n \xrightarrow{H\text{-converges}} M, \quad (2.13)$$

where $M \in L_+(\mathbb{R}^N, \mathbb{R}^N)$ is a positive definite matrix equivalent to A .

We have the following integral representation similar to (2.3):

$$\begin{aligned} M e_k \cdot e_l = m_{kl} &= \frac{1}{|\omega|} \int_\omega A_\omega(y) \nabla w_{e_k}(y) \cdot \nabla w_{e_l}(y) \, dy \\ &= \frac{1}{|\omega|} \int_\omega A_\omega(y) \nabla w_{e_k}(y) \cdot e_l \, dy, \end{aligned} \quad (2.14)$$

where w_{e_k}, w_{e_l} are the solution of (2.8) for $\lambda = e_k$ and $\lambda = e_l$, respectively. \square

Example 2.1. (Spherical Inclusions in two-phase medium) If $\omega = B(0, 1) = \{y \mid |y| \leq 1\}$ and

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

α and β are known as core and coating, respectively. Then A_ω is equivalent to γI , where γ satisfies

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

Example 2.2. (Elliptical Inclusions in two-phase medium [19]) For $m_1, \dots, m_N \in \mathbb{R}$ and $\rho + m_j > 0$ for $j = 1, \dots, N$, the family of confocal ellipsoids S_ρ of equation

$$\sum_{j=1}^N \frac{y_j^2}{\rho + m_j} = 1$$

defines implicitly a real function ρ , outside a possibly degenerate ellipsoid in a subspace of dimension $< N$.

Now, if we consider $\omega = E_{\rho_2+m_1, \dots, \rho_2+m_N} = \left\{ y \mid \sum_{j=1}^N \frac{y_j^2}{\rho_2+m_j} \leq 1 \right\}$, with $\rho_2 + \min_j m_j > 0$ and

$$A_\omega(y) = a_E(\rho)I = \begin{cases} \alpha I & \text{if } \rho \leq \rho_1, \\ \beta I & \text{if } \rho_1 < \rho \leq \rho_2, \end{cases}$$

then A_ω is equivalent to a constant diagonal matrix $\Gamma = [\gamma_{jj}]_{1 \leq j \leq N}$ satisfying

$$\sum_{j=1}^N \frac{1}{\beta - \gamma_{jj}} = \frac{(1 - \theta)\alpha + (N + \theta - 1)\beta}{\theta\beta(\beta - \alpha)}, \quad \text{with } \theta = \prod_j \sqrt{\frac{\rho_1 + m_j}{\rho_2 + m_j}}.$$

□

Bloch waves, Bloch eigenvalues and eigenvectors associated with the Hashin–Shtrikman structures

Let $\omega \subset \mathbb{R}^N$ be a bounded open domain with Lipschitz boundary and $A_\omega(y) = [a_{kl}^\omega(y)]_{1 \leq k, l \leq N} \in \mathcal{M}(\alpha, \beta, \omega)$. We consider the following spectral problem parameterized by $\eta \in \mathbb{R}^N$: find $\lambda_\omega := \lambda_\omega(\eta) \in \mathbb{C}$ and $\varphi_\omega := \varphi_\omega(y; \eta)$ (not identically zero) such that

$$\begin{aligned} \mathcal{A}_\omega(\eta)\varphi_\omega(y; \eta) &= -\left(\frac{\partial}{\partial y_k} + i\eta_k\right) \left[a_{kl}^\omega(y) \left(\frac{\partial}{\partial y_l} + i\eta_l\right) \right] \varphi_\omega(y; \eta) \\ &= \lambda_\omega(\eta)\varphi_\omega(y; \eta) \text{ in } \omega, \end{aligned} \tag{2.15}$$

$$\varphi_\omega(y; \eta) \text{ is constant on } \partial\omega \text{ and } \int_{\partial\omega} a_{kl}^\omega(y) \left(\frac{\partial}{\partial y_l} + i\eta_l\right) \varphi_\omega(y; \eta) \nu_k \, d\sigma = 0,$$

where ν is the outer normal vector on the boundary and $d\sigma$ is the surface measure on $\partial\omega$.

We introduce the state spaces of the above spectral problem:

$$\begin{aligned} L_c^2(\omega) &= \{\varphi \in L_{loc}^2(\mathbb{R}^N) \mid \varphi \text{ is constant in } \mathbb{R}^N \setminus \omega\}, \\ H_c^1(\omega) &= \{\varphi \in H_{loc}^1(\mathbb{R}^N) \mid \varphi \text{ is constant in } \mathbb{R}^N \setminus \omega\} \\ &= \{\varphi \in H^1(\omega) \mid \varphi|_{\partial\omega} = \text{constant}\}. \end{aligned}$$

Here, c is a floating constant depending on the element under consideration. $L_c^2(\omega)$ and $H_c^1(\omega)$ are proper subspace of $L^2(\omega)$ and $H^1(\omega)$ respectively, and they inherit the subspace norm-topology of the parent space.

Prior to that, we have this following result establishing the existence of the Bloch eigenlements:

Proposition 2.2. (Existence result [4]) *Fix $\eta \in \mathbb{R}^N$. Then, there exist a sequence of eigenvalues $\{\lambda_{\omega,m}(\eta); m \in \mathbb{N}\}$ and its corresponding eigenvectors $\{\varphi_{\omega,m}(y; \eta) \in H_c^1(\omega), m \in \mathbb{N}\}$ such that*

- (i) $\mathcal{A}_\omega(\eta)\varphi_{\omega,m}(y; \eta) = \lambda_{\omega,m}(\eta)\varphi_{\omega,m}(y; \eta) \quad \forall m \in \mathbb{N}$.
- (ii) $0 \leq \lambda_{\omega,1}(\eta) \leq \lambda_{\omega,2}(\eta) \leq \dots \rightarrow \infty$; each eigenvalue is of finite multiplicity.
- (iii) $\{\varphi_{\omega,m}(\cdot; \eta); m \in \mathbb{N}\}$ is an orthonormal basis for $L_c^2(\omega)$.
- (iv) For ϕ in the domain of $\mathcal{A}_\omega(\eta)$, we have

$$\mathcal{A}_\omega(\eta)\phi(y) = \sum_{m=1}^{\infty} \lambda_{\omega,m}(\eta)(\phi, \varphi_{\omega,m}(\cdot; \eta))\varphi_{\omega,m}(y; \eta).$$

As the eigen-branch emanating from the first eigenvalue plays the key role, we concentrate only for $m = 1$ to have the following regularity properties:

Proposition 2.3. (Regularity of the ground state [4]) *Let $\lambda_{\omega,1}(\eta), \varphi_{\omega,1}(\cdot; \eta)$ be the first eigenvalue and the first eigenvector of the spectral problem defined in (2.15). Then, there exists a neighborhood ω' around zero such that*

$$\eta \longmapsto (\lambda_{\omega,1}(\eta), \varphi_{\omega,1}(\cdot; \eta)) \in \mathbb{C} \times H_c^1(\omega) \text{ is analytic on } \omega'.$$

At $\eta = 0$, $\lambda_{\omega,1}(0)$ is simple. There is a choice of the first eigenvector $\varphi_{\omega,1}(y; \eta)$ satisfying

$$\varphi_{\omega,1}(y; \eta) = \frac{1}{|\omega|^{1/2}} \quad \forall y \in \partial\omega \text{ and } \forall \eta \in \omega'.$$

Moreover, we have the following relations:

$$\begin{aligned} \lambda_{\omega,1}(0) = 0, \quad D_k \lambda_{\omega,1}(0) &= \frac{\partial \lambda_{\omega,1}}{\partial \eta_k}(0) = 0 \quad \forall k = 1, \dots, N, \\ \varphi_{\omega,1}(\cdot; 0) = |\omega|^{-1/2}, \quad D_k \varphi_{\omega,1}(y, 0) &= i|\omega|^{-1/2}(w_{e_k}(y) - y_k), \quad (2.16) \\ \frac{1}{2} D_{kl}^2 \lambda_{\omega,1}(0) &= \frac{1}{2} \frac{\partial^2 \lambda_{\omega,1}}{\partial \eta_k \partial \eta_l}(0) = m_{kl} \quad \forall k, l = 1, \dots, N, \end{aligned}$$

where the last expression is considered as a Bloch spectral representation of the homogenized tensor. \square

Moreover, all odd order derivatives of $\lambda_{\omega,1}$ at $\eta = 0$ are zero, that is

$$D^q \lambda_{\omega,1}(0) = 0 \quad \forall q \in \mathbb{Z}_+^N, |q| \text{ odd}. \quad (2.17)$$

In particular, the third order derivative is zero. However, we are interested in the further next order approximation by calculating the fourth order derivatives of $\lambda_{\omega,1}(0)$, that is $D_{klmn}^4 \lambda_{\omega,1}(0)$, which is in general a non-positive definite tensor and can be defined as follows: the second order derivative of the eigenvector $D_{kl}^2 \varphi_{\omega,1}(\cdot; 0) \in H_0^1(\omega)$ solves

$$\begin{aligned} \mathcal{A} D_{kl}^2 \varphi_{\omega,1}(y; 0) &= -(a_{kl}^\omega(y) - m_{kl})\varphi_{\omega,1}(y; 0) - i C_k(D_l(\varphi_{\omega,1}(y; 0))) \\ &\quad - i C_l(D_k \varphi_{\omega,1}(y; 0)) \text{ in } \omega, \end{aligned} \quad (2.18)$$

$$D_{kl}^2 \varphi_{\omega,1}(y; 0) = 0 \text{ on } \partial\omega \text{ and } \int_{\partial\omega} A_\omega(y) \nabla_y D_{kl}^2 \varphi_{\omega,1}(y; 0) \cdot \nu \, d\sigma = 0.$$

We call $D_{kl}^2 \varphi_{\omega,1}(y; 0) = |\omega|^{-1/2} w_{kl}(y)$ and let us define

$$X_{\omega}^{(1)} = \eta_k(w_{e_k}(y) - y_k) \text{ and } X_{\omega}^{(2)} = \eta_k \eta_l w_{kl} \text{ likewise in (2.5).}$$

Then, by summation, following [7, Proposition 3.2] it can be shown that the following expression defines the fourth order derivative of $\lambda_{\omega,1}(\eta)$ at $\eta = 0$:

$$\begin{aligned} \frac{1}{4!} D_{klmn}^4 \lambda_{\omega,1}(0) \eta_k \eta_l \eta_m \eta_n &= -\frac{1}{|\omega|} \int_{\omega} \mathcal{A} \left(X_{\omega}^{(2)} - \frac{1}{2} (X_{\omega}^{(1)})^2 \right) \cdot \left(X_{\omega}^{(2)} - \frac{1}{2} (X_{\omega}^{(1)})^2 \right) dy \\ &\leq 0. \end{aligned} \tag{2.19}$$

This tells us that $\lambda_{\omega,1}^{(4)}(\eta)$ at $\eta = 0$ is a non-positive definite tensor. \square

Next, we consider a medium in Ω with Hashin–Shtrikman micro-structures. Let us introduce the operator \mathcal{A}_{ω}^n governed with the Hashin–Shtrikman construction:

$$\begin{aligned} \mathcal{A}_{\omega}^n &= -\frac{\partial}{\partial x_k} \left(a_{kl}^n(x) \frac{\partial}{\partial x_l} \right) \text{ with } a_{kl}^n(x) \\ &= a_{kl}^{\omega} \left(\frac{x - y^{p,n}}{\varepsilon_{p,n}} \right) \text{ in } (\varepsilon_{p,n}\omega + y^{p,n}) \text{ almost everywhere on } \Omega, \end{aligned} \tag{2.20}$$

where $meas(\Omega \setminus \cup_{p \in K} (\varepsilon_{p,n}\omega + y^{p,n})) = 0$, with $\kappa_n = \sup_{p \in K} \varepsilon_{p,n} \rightarrow 0$ for a finite or countable K and, for each n , the sets $(\varepsilon_{p,n}\omega + y^{p,n})$, $p \in K$ are disjoint.

We obtain the spectral resolution of \mathcal{A}_{ω}^n for fixed n , in each $\{\varepsilon_{p,n}\omega + y^{p,n}\}_{p \in K}$ domain, in an analogous manner. We introduce the shifted operator

$$\begin{aligned} (\mathcal{A}_{\omega}^{n,p})(\xi) &= -\left(\frac{\partial}{\partial x_k} + i\xi_k \right) \left(a_{kl}^{\omega} \left(\frac{x - y^{p,n}}{\varepsilon_{p,n}} \right) \left(\frac{\partial}{\partial x_l} + i\xi_l \right) \right), \\ x &\in (\varepsilon_{p,n}\omega + y^{p,n}). \end{aligned} \tag{2.21}$$

By homothety, for a fixed n and for each p , we define the first Bloch eigenvalue $\lambda_{\omega,1}^{n,p}(\xi)$ and the corresponding Bloch mode $\varphi_{\omega,1}^{n,p}(\cdot; \xi)$ for the operator $(\mathcal{A}_{\omega}^{n,p})(\xi)$ for $\xi \in \kappa_n^{-1} \omega'$ as follows:

$$\begin{aligned} \lambda_{\omega,1}^{n,p}(\xi) &:= \varepsilon_{p,n}^{-2} \lambda_{\omega,1}(\varepsilon_{p,n}\xi), \\ \varphi_{\omega,1}^{n,p}(x; \xi) &:= \varphi_{\omega,1} \left(\frac{x - y^{p,n}}{\varepsilon_{p,n}}; \varepsilon_{p,n}\xi \right), \quad x \in (\varepsilon_{p,n}\omega + y^{p,n}), \end{aligned} \tag{2.22}$$

where $\lambda_{\omega,1}(\eta)$ and $\varphi_{\omega,1}(y; \eta)$ are the eigenlements defined in Proposition 2.2. This leads to define the Bloch transformation in $L^2(\mathbb{R}^N)$ in the following manner:

Proposition 2.4. (Bloch transformation [4])

1. For $g \in L^2(\mathbb{R}^N)$, for each n , the following limit in $L^2(\kappa_n^{-1} \omega')$ space exists:

$$\begin{aligned} B_1^n g(\xi) &:= B_1^{(\varepsilon_{p,n}, y^{p,n})} g(\xi) \\ &:= \sum_p \int_{\varepsilon_{p,n}\omega + y^{p,n}} g(x) e^{-ix \cdot \xi} \overline{\varphi_{\omega,1} \left(\frac{x - y^{p,n}}{\varepsilon_{p,n}}; \varepsilon_{p,n}\xi \right)} dx, \end{aligned} \tag{2.23}$$

where, for each n , $\text{meas}(\mathbb{R}^N \setminus \bigcup_{p \in K} (\varepsilon_{p,n}\omega + y^{p,n})) = 0$, with $\kappa_n = \sup_{p \in K} \varepsilon_{p,n} \rightarrow 0$ for a finite or countable K and the sets $(\varepsilon_{p,n}\omega + y^{p,n})$, $p \in K$ are disjoint. The above definition (2.23) is the corresponding first Bloch transformation governed with Hashin–Shtrikman micro-structures.

2. We have the following Bessel inequality for elements of $L^2(\mathbb{R}^N)$:

$$\int_{\kappa_n^{-1}\omega'} |B_1^n g(\xi)|^2 d\xi \leq \mathcal{O}(1) \|g\|_{L^2(\mathbb{R}^N)}^2. \tag{2.24}$$

3. For $g \in H^1(\mathbb{R}^N)$, we have

$$B_1^n (\mathcal{A}_\omega^n g(\xi)) := \sum_p \int_{\varepsilon_{p,n}\omega + y^{p,n}} \lambda_{\omega,1}^{n,p} g(x) e^{-ix \cdot \xi} \varphi_{\omega,1} \left(\frac{x - y^{p,n}}{\varepsilon_{p,n}}; \varepsilon_{p,n} \xi \right) dx. \tag{2.25}$$

One has the first Bloch transform is an approximation to the Fourier transform.

Proposition 2.5. (First Bloch transform tends to Fourier transform [4])

1. If $g_n \rightharpoonup g$ in $L^2(\mathbb{R}^N)$ weak, then $\chi_{\kappa_n^{-1}\omega'}(\xi) B_1^n g^n(\xi) \rightharpoonup \widehat{g}(\xi)$ in $L^2(\mathbb{R}^N)$ weak, provided there is a fixed compact R such that support of $g^n \subseteq R \quad \forall n$.
2. If $g_n \rightarrow g$ in $L^2(\mathbb{R}^N)$ strong, then for the subsequence $\varepsilon_{p,n}$, $\chi_{\kappa_n^{-1}\omega'}(\xi) B_1^n g^n \rightarrow \widehat{g}(\xi)$ in $L^2_{loc}(\mathbb{R}^N)$.

Using these above tools the following homogenization theorem has been deduced in [4]:

Theorem 2.1. (Homogenization result [4]) *Let us consider Ω be an open subset of \mathbb{R}^N and consider the operator \mathcal{A}_ω^n introduced in (2.20) governed with the Hashin–Shtrikman construction, where the matrix $A_\omega \in \mathcal{M}(\alpha, \beta; \omega)$ is equivalent to M in the sense of (2.8). Let $f \in L^2(\Omega)$ and consider $u^n \in H_0^1(\Omega)$ being the unique solution of the boundary value problem*

$$\mathcal{A}_\omega^n u^n = f \quad \text{in } \Omega.$$

Then, there exists $u \in H_0^1(\Omega)$ such that the sequence u^n converges to u in $H_0^1(\Omega)$ weak, with the following convergence of the flux:

$$\sigma_\omega^n = A_\omega^n \nabla u^n \rightharpoonup M \nabla u = \sigma_\omega \quad \text{in } L^2(\Omega) \text{ weak.}$$

In particular, the limit u satisfies homogenized equation

$$\mathcal{A}_\omega^* u = - \frac{\partial}{\partial x_l} \left(m_{kl} \frac{\partial}{\partial x_k} u \right) = f \quad \text{in } \Omega.$$

□

We end our discussion here concerning with the homogenized matrix. In the next section we will move into defining the dispersion tensor for the Hashin–Shtrikman micro-structures.

3. Dispersion Tensor and Hashin–Shtrikman Structures

Here we are going to define the dispersion tensor or the *Burnett coefficient*, more precisely, the fourth order approximation of the medium governed by the Hashin–Shtrikman micro-structures, while in the previous section we have studied the homogenized coefficient as a second order approximation of the medium. Let us consider Ω be an open subset of \mathbb{R}^N . We recall (2.20) where we have introduced the operator \mathcal{A}_ω^n governed with the Hashin–Shtrikman construction

$$\mathcal{A}_\omega^n = -\frac{\partial}{\partial x_k} \left(a_{kl}^n(x) \frac{\partial}{\partial x_l} \right),$$

with $A_\omega^n(x) = [a_{kl}^n(x)] = \left[a_{kl}^\omega \left(\frac{x-y^{p,n}}{\varepsilon_{p,n}} \right) \right]$ in $(\varepsilon_{p,n}\omega + y^{p,n})$, almost everywhere on Ω , where $meas(\Omega \setminus \cup_{p \in K} (\varepsilon_{p,n}\omega + y^{p,n})) = 0$, with $\kappa_n = \sup_{p \in K} \varepsilon_{p,n} \rightarrow 0$ for a finite or countable K and, for each n , the sets $(\varepsilon_{p,n}\omega + y^{p,n})$, $p \in K$ are disjoint. Previously, for each n , we restricted the operator \mathcal{A}_ω^n in each $\{\varepsilon_{p,n}\omega + y^{p,n}\}_{p \in K}$ to define $\mathcal{A}_\omega^{n,p}$. Then, by homothecy, we obtained its first Bloch spectral data $(\lambda_{\omega,1}^{n,p}, \varphi_{\omega,1}^{n,p})$ in (2.22). We have the following Taylor expansion around zero:

$$\begin{aligned} \lambda_{\omega,1}^{n,p}(\xi) &= \frac{1}{2!} \frac{\partial^2 \lambda_{\omega,1}}{\partial \eta_k \partial \eta_l}(0) \xi_k \xi_l + \varepsilon_{p,n}^2 \frac{1}{4!} \frac{\partial^4 \lambda_{\omega,1}}{\partial \eta_k \partial \eta_l \partial \eta_m \partial \eta_n}(0) \xi_k \xi_l \xi_m \xi_n + o(\varepsilon_{p,n}^2) \\ &= m_{kl} \xi_k \xi_l + \varepsilon_{p,n}^2 \frac{1}{4!} \frac{\partial^4 \lambda_{\omega,1}}{\partial \eta_k \partial \eta_l \partial \eta_m \partial \eta_n}(0) \xi_k \xi_l \xi_m \xi_n + o(\varepsilon_{p,n}^2), \quad \xi \in \kappa_n^{-1} \omega'. \end{aligned}$$

The first term in the above expression is providing the homogenized medium as the second order approximation. The second term provides the next order that is the fourth order approximation of the medium by considering the last term to be sufficiently small enough. As we know, for each n depending upon the parameter p , the scales $\varepsilon_{p,n}$ could vary in plenty of ways with remaining inside the class of sequences of Vitali coverings of Ω . The second order approximation or the homogenized tensor $m_{kl} \xi_k \xi_l$ is universal among all possible Vitali coverings, whereas the fourth order approximation is not so. There is a more vibrant dependence on the scales $\varepsilon_{p,n}$, and it varies over the Vitali coverings. Taking into account this fact, in order to define the *Burnett coefficient* or the dispersion tensor d_{HS} in the class of generalized Hashin–Shtrikman structures, we will introduce an approximating quantity d_{HS}^n by taking an average over the various scales $\varepsilon_{p,n}^2$ and then, quotient it out by the highest scale factor κ_n^2 ($\kappa_n = \sup_{p \in K} \varepsilon_{p,n}$). For that, we will consider

the first Bloch eigenvalue associated with the shifted operator $\mathcal{A}_\omega^n(\xi)$ ($\xi \in \mathbb{R}^N$) in Ω . Finally, by passing to the limit as $n \rightarrow \infty$, we will characterize the dispersion tensor d_{HS} for the medium.

We begin by introducing the following spectral problem in Ω associated with the shifted operator $\mathcal{A}^n(\xi)$ ($\xi \in \mathbb{R}^N$) likewise in (2.15): for each fixed $n \in \mathbb{N}$,

$$\begin{aligned} \mathcal{A}^n_\omega(\xi)\varphi^n_\Omega(x; \xi) &= -\left(\frac{\partial}{\partial x_k} + i\xi_k\right)\left[a^n_{kl}(x)\left(\frac{\partial}{\partial x_l} + i\xi_l\right)\right]\varphi^n_\Omega(x; \xi) \\ &= \lambda^n_\Omega(\xi)\varphi^n_\Omega(x; \xi) \text{ in } \Omega, \end{aligned} \tag{3.1}$$

$$\varphi^n_\Omega(x; \xi) \text{ is constant on } \partial\Omega \text{ and } \int_{\partial\Omega} a^n_{kl}(x)\left(\frac{\partial}{\partial x_l} + i\xi_l\right)\varphi^n_\Omega(x; \xi)\nu_k \, d\sigma = 0,$$

where ν is the outer normal vector on the boundary and $d\sigma$ is the surface measure on $\partial\Omega$.

Weak formulation: Here first we introduce the function spaces

$$\begin{aligned} L^2_c(\Omega) &= \{\varphi \in L^2_{loc}(\mathbb{R}^N) \mid \varphi \text{ is constant in } \mathbb{R}^N \setminus \Omega\}, \\ H^1_c(\Omega) &= \{\varphi \in H^1_{loc}(\mathbb{R}^N) \mid \varphi \text{ is constant in } \mathbb{R}^N \setminus \Omega\}. \end{aligned}$$

Here c is a floating constant depending on the element under consideration.

As a next step we give the weak formulation of the problem in these function spaces. We are interested in proving the existence of the eigenvalue and the corresponding eigenvector $(\lambda^n_\Omega(\eta), \varphi^n_\Omega(x; \xi)) \in \mathbb{C} \times H^1_c(\Omega)$ of the following weak formulation of (3.1): for each fixed n ,

$$\begin{aligned} \int_\Omega a^n_{kl}(x)\left(\frac{\partial\varphi^n_\Omega(x; \xi)}{\partial x_l} + i\xi_l\varphi^n_\Omega(x; \xi)\right)\overline{\left(\frac{\partial\psi}{\partial x_k} + i\xi_k\psi\right)} \, dx \\ = \lambda^n_\Omega(\xi) \int_\Omega \varphi^n_\Omega(x; \xi)\overline{\psi} \, dx \quad \forall \psi \in H^1_c(\Omega). \end{aligned} \tag{3.2}$$

Existence Result: By following the same analysis presented in [4], we state the corresponding existence result for the problem (3.2).

Proposition 3.1. *Fix $\xi \in \mathbb{R}^N$. For each fixed n , there exist a sequence of eigenvalues $\{\lambda^n_{\Omega,m}(\xi) \geq 0; m \in \mathbb{N}\}$ and its corresponding eigenvectors $\{\varphi^n_{\Omega,m}(x; \xi) \in H^1_c(\Omega); m \in \mathbb{N}\}$ satisfying (3.2).*

Regularity of the ground state: In the next proposition, we announce the regularity result of ground state based on the Kato–Rellich analysis which has been done in [4].

Proposition 3.2. *For each fixed $n \in \mathbb{N}$, we have that*

1. *Zero is the first eigenvalue of (3.2) at $\xi = 0$ and it is an isolated point of the spectrum with its algebraic multiplicity equal to one.*
2. *There exists an open neighborhood Ω'_n around zero such that the first eigenvalue $\lambda^n_{\Omega,1}(\xi)$ is an analytic function on Ω'_n and there is a choice of the first eigenvector $\varphi^n_{\Omega,1}(x; \xi)$ satisfying*

$$\xi \longmapsto \varphi^n_{\Omega,1}(\cdot; \xi) \in H^1_c(\Omega) \text{ is analytic on } \Omega'_n \text{ and } \varphi^n_{\Omega,1}(x; 0) = |\Omega|^{-1/2},$$

with the boundary normalization condition

$$\varphi_{\omega,1}(y; \eta) = \frac{1}{|\omega|^{1/2}} \quad \forall y \in \partial\omega \text{ and } \forall \eta \in \omega'.$$

Derivatives of $\lambda_{\Omega,1}^n(\xi)$ and $\varphi_{\Omega,1}^n(\xi)$ at $\xi = 0$: The procedure consists of differentiating the eigenvalue equation (3.1) for $\lambda_{\omega}^n(\xi) = \lambda_{\omega,1}^n(\xi)$ and $\varphi_{\omega}^n(\cdot; \xi) = \varphi_{\Omega,1}^n(\cdot; \xi)$.

Step 1. Zeroth order derivatives: We simply recall that $\varphi_{\Omega,1}^n(x; 0) = |\Omega|^{-1/2}$, by our choice, and $\lambda_{\Omega,1}^n(0) = 0$.

Step 2. First order derivatives of $\lambda_{\Omega,1}^n(\xi)$ at $\xi = 0$: Differentiating the equation (3.1) once with respect to ξ_k and then taking scalar product with $\varphi_{\Omega,1}^n(\cdot; \xi)$ in $L^2(\Omega)$ at $\xi = 0$, we get

$$\langle D_k(\mathcal{A}_{\omega}^n(0) - \lambda_{\Omega,1}^n(0))\varphi_{\Omega,1}^n(\cdot; 0), \varphi_{\Omega,1}^n(\cdot; 0) \rangle = 0.$$

Then, using the fact that

$$\begin{aligned} D_k \mathcal{A}_{\omega}^n(0)\varphi_{\Omega,1}^n(\cdot; 0) &= iC_k^n(\varphi_{\Omega,1}^n(\cdot; 0)) \\ &= -a_{kj}^n(x) \frac{\partial}{\partial x_j}(\varphi_{\Omega,1}^n(\cdot; 0)) - \frac{\partial}{\partial x_j}(a_{kj}^n(x)\varphi_{\Omega,1}^n(\cdot; 0)) \\ &= -\frac{\partial}{\partial x_j}(a_{kj}^n(x)\varphi_{\Omega,1}^n(\cdot; 0)), \end{aligned}$$

whose integral over Ω vanishes through integration by parts together with using the boundary conditions in (3.1), it follows that

$$D_k \lambda_{\Omega,1}^n(0) = 0 \quad \forall k = 1, \dots, N. \tag{3.3}$$

Step 3. First order derivatives of $\varphi_{\Omega,1}^n(\cdot; \xi)$ at $\xi = 0$: By differentiating (3.1) once with respect to ξ_k at zero, one has

$$A_{\omega}^n(D_k \varphi_{\Omega,1}^n(\cdot; 0)) = -\frac{\partial}{\partial x_j}(a_{kj}^n(x)\varphi_{\Omega,1}^n(\cdot; 0)) \quad \text{in } \Omega, \tag{3.4}$$

$$D_k \varphi_{\Omega,1}^n(\cdot; 0) = 0 \quad \text{on } \partial\Omega \tag{3.5}$$

$$\text{and } \int_{\partial\Omega} A_{\omega}^n(x) (\nabla_x D_k \varphi_{\Omega,1}^n(\cdot; 0) + i\varphi_{\Omega,1}^n(\cdot; 0)e_k) \cdot \nu \, d\sigma = 0. \tag{3.6}$$

As we can see along with boundary condition (3.5) for the elliptic equation (3.4), the solution $D_k \varphi_{\Omega,1}^n(\cdot; 0)$ gets uniquely determined, and the condition (3.6) is consistent as it comes via integrating the equation (3.4). By comparing with (2.11), let us define

$$D_k \varphi_{\Omega,1}^n(x; 0) = \begin{cases} i|\Omega|^{-1/2} \varepsilon_{p,n}(w_{ek}(\frac{x-y^{p,n}}{\varepsilon_{p,n}}) - (e_k, \frac{x-y^{p,n}}{\varepsilon_{p,n}})) & \text{in } (\varepsilon_{p,n}\omega + y^{p,n}) \\ 0 & \text{otherwise.} \end{cases} \tag{3.7}$$

Then, clearly $D_k \varphi_{\Omega,1}^n(\cdot; 0) \in H^1(\Omega)$ satisfies (3.5). We also notice that (3.7) solves the equation (3.4) in each $\{\varepsilon_{p,n}\omega + y^{p,n}\}_{p \in K}$. In order to show it solves (3.4) in entire Ω , we need to prove that

$$\int_{\Omega} A_{\omega}^n(x) (\nabla_x D_k \varphi_{\Omega,1}^n(x; 0) + i\varphi_{\Omega,1}^n(x; 0)e_k) \cdot \nabla_x \varphi(x) \, dx = 0 \quad \forall \varphi \in \mathcal{D}(\Omega). \tag{3.8}$$

We have that

$$\begin{aligned} & \int_{\Omega} A_{\omega}^n(x) (\nabla_x D_k \varphi_{\Omega,1}^n(x; 0) + i \varphi_{\Omega,1}^n(x; 0) e_k) \cdot \nabla_x \varphi(x) dx \\ &= \frac{i}{|\Omega|^{1/2}} \sum_p \varepsilon_{p,n}^{N-1} \int_{\omega} A_{\omega}(y) \nabla_y w_{e_k}(y) \cdot \nabla_y \varphi_p(y) dy, \end{aligned} \tag{3.9}$$

where $y = \frac{x - y^{p,n}}{\varepsilon_{p,n}} \in \omega$ whenever $x \in (\varepsilon_{p,n}\omega + y^{p,n})$ and $\varphi_p(y) = \varphi(\varepsilon_{p,n}y + y^{p,n})$ with $\nabla_y \varphi_p(y) = \varepsilon_{p,n} \nabla_x \varphi(x)$. Then, doing integration by parts on the right hand side of (3.9) together with using (2.8), we get

$$\begin{aligned} & \int_{\Omega} A_{\omega}^n(x) (\nabla_x D_k \varphi_{\Omega,1}^n(x; 0) + i \varphi_{\Omega,1}^n(x; 0) e_k) \cdot \nabla_x \varphi(x) dx \\ &= \frac{i}{|\Omega|^{1/2}} \sum_p \varepsilon_{p,n}^{N-1} \int_{\partial\omega} M e_k \cdot \nu \varphi_p(y) d\sigma \\ &= \frac{i}{|\Omega|^{1/2}} M e_k \cdot \sum_p \varepsilon_{p,n}^{N-1} \int_{\omega} \nabla_z \varphi_p(y) dy \\ &= \frac{i}{|\Omega|^{1/2}} M e_k \cdot \int_{\Omega} \nabla_x \varphi(x) dx \\ &= 0 \quad \forall \varphi \in \mathcal{D}(\Omega). \end{aligned}$$

Thus $D_k \varphi_{\Omega,1}^n(x; 0)$ is rightly defined in (3.7) to satisfy (3.4), (3.5), (3.6) uniquely.

Step 4. Second derivatives of $\lambda_{\Omega,1}^n(\xi)$ at $\xi = 0$: By differentiating (3.1) twice with respect to ξ_k and ξ_l , respectively and then taking scalar product with $\varphi_{\Omega,1}^n(\cdot; \xi)$ in $L^2(\Omega)$ at $\xi = 0$, we get

$$\begin{aligned} & (D_{kl}^2(\mathcal{A}_{\omega}^n(0) - \lambda_{\Omega,1}^n(0)) \varphi_{\Omega,1}^n(\cdot; 0), \varphi_{\Omega,1}^n(\cdot; 0)) \\ &+ ([D_k(\mathcal{A}_{\omega}^n(0) - \lambda_{\Omega,1}^n(0))] D_l \varphi_{\Omega,1}^n(\cdot; 0), \varphi_{\Omega,1}^n(\cdot; 0)) \\ &+ ([D_l(\mathcal{A}_{\omega}^n(0) - \lambda_{\Omega,1}^n(0))] D_k \varphi_{\Omega,1}^n(\cdot; 0), \varphi_{\Omega,1}^n(\cdot; 0)) = 0. \end{aligned}$$

By using the information obtained in the previous steps, we get

$$\begin{aligned} \frac{1}{2} D_{kl}^2 \lambda_{\Omega,1}^n(0) &= \frac{1}{|\Omega|} \int_{\Omega} a_{kl}^n(x) dx \\ &\quad - \frac{1}{2|\Omega|} \int_{\Omega} [C_k^n(D_l \varphi_{\Omega,1}^n(x; 0)) + C_l^n(D_k \varphi_{\Omega,1}^n(x; 0))] dx \\ &= \frac{1}{2|\Omega|} \sum_p \int_{\varepsilon_{p,n}\omega + y^{p,n}} A_{\omega}\left(\frac{x - y^{p,n}}{\varepsilon_{p,n}}\right) \left(\nabla w_{e_k}\left(\frac{x - y^{p,n}}{\varepsilon_{p,n}}\right) \cdot e_l \right. \\ &\quad \left. + \nabla w_{e_l}\left(\frac{x - y^{p,n}}{\varepsilon_{p,n}}\right) \cdot e_k\right) dx \\ &= \frac{1}{2} \int_{\omega} A_{\omega}(y) (\nabla_y w_{e_k}(y) \cdot e_l + \nabla_y w_{e_l}(y) \cdot e_k) dy \\ &= m_{kl} \quad \forall k, l = 1, \dots, N, \end{aligned}$$

due to the integral identity (2.14), which are indeed the homogenized coefficients governed with the Hashin–Shtrikman constructions. We see that $\frac{1}{2}D_{kl}^2\lambda_{\Omega,1}^n(0)$ is independent of n . Thus, it does not depend on the choice of translations $y^{p,n}$ and the scales $\varepsilon_{p,n}$ as long as they are bound to satisfy the Vitali covering criteria (2.9).

Step 5. Higher order derivatives: In general, the process can be continued indefinitely to compute all derivatives of $\lambda_{\Omega,1}^n(\xi)$ and $\varphi_{\Omega,1}^n(\cdot; \xi)$ at $\xi = 0$. In particular, the third order derivative is zero, that is $D^q\lambda_{\Omega,1}^n(0) = 0$, $|q| = 3$. However, we are interested in the fourth order derivatives of $\lambda_{\Omega,1}^n(0)$, that is $D_{klmn}^4\lambda_{\Omega,1}^n(0)$, which is in general a non-positive definite tensor and can be defined as follows: the second order derivative of the eigenvector $D_{kl}^2\varphi_{\Omega,1}^n(\cdot; 0) \in H_0^1(\Omega)$ solves

$$\begin{aligned} A_\omega^n D_{kl}^2\varphi_{\Omega,1}^n(x; 0) &= -(a_{kl}^n(x) - m_{kl})\varphi_{\Omega,1}^n(x; 0) - iC_k^n(D_l(\varphi_{\Omega,1}^n(x; 0)) \\ &\quad - iC_l(D_k\varphi_{\Omega,1}^n(x; 0))) \text{ in } \Omega, \tag{3.10} \\ D_{kl}^2\varphi_{\Omega,1}^n(x; 0) &= 0 \text{ on } \partial\Omega \text{ and } \int_{\partial\Omega} A_\omega^n(x)\nabla_x D_{kl}^2\varphi_{\Omega,1}^n(x; 0) \cdot \nu \, d\sigma = 0. \end{aligned}$$

The above equation (3.10) has a unique solution that we would like to define as

$$D_{kl}^2\varphi_{\Omega,1}^n(x; 0) = \begin{cases} |\Omega|^{-1/2} \varepsilon_{p,n}^2 \tilde{w}_{kl}\left(\frac{x-y^{p,n}}{\varepsilon_{p,n}}\right) & \text{in } \varepsilon_{p,n}\omega + y^{p,n}, \\ 0 & \text{otherwise,} \end{cases} \tag{3.11}$$

where \tilde{w}_{kl} is defined likewise by (2.8) as follows: after extending $A_\omega \in \mathcal{M}(\alpha, \beta; \omega)$ by $A_\omega(x) = M$ for $x \in \mathbb{R}^N \setminus \omega$, $\tilde{w}_{kl} \in H^1(\mathbb{R}^N)$ satisfies

$$\begin{aligned} -\operatorname{div}(A_\omega \nabla \tilde{w}_{kl}(x)) &= -(a_{kl}^\omega(x) - m_{kl}) - iC_k^\omega(w_{e_l}(x) - x_l) \\ &\quad - iC_l^\omega(w_{e_k}(x) - x_k) \text{ in } \mathbb{R}^N, \tag{3.12} \\ \tilde{w}_{kl}(x) &= 0 \text{ in } \mathbb{R}^N \setminus \omega, \end{aligned}$$

where $C_k^\omega(\varphi) = -a_{kj}^\omega(x)\frac{\partial\varphi}{\partial x_j} - \frac{\partial}{\partial x_j}(a_{kj}^\omega(x)\varphi)$.

If such $\tilde{w}_{kl} \in H^1(\mathbb{R}^N)$ exists $\forall k, l = 1, \dots, N$, then following the same arguments presented in Step 3, $D_{kl}^2\varphi_{\Omega,1}^n(\cdot; 0)$ defined in (3.11) belongs to $H_0^1(\Omega)$ and solves (3.10) in Ω .

Notice that $w_{kl} \in H_0^1(\omega)$ defined in (2.18) and $\tilde{w}_{kl} \in H_0^1(\omega)$ solves the same equation (3.12). The only difference occurs in the co-normal derivative of \tilde{w} on $\partial\omega$, because we have

$$\nabla \tilde{w}_{kl}(x) \cdot \nu = 0 \text{ on } \partial\omega.$$

In the next section (cf. Proposition 4.1 below), we show that in the case of two-phase spherical inclusions (see Example 2.1) such \tilde{w}_{kl} exists and is equal to w_{kl} for each $k, l = 1, \dots, N$.

We further define

$$X_{\Omega,1}^n = -i|\Omega|^{1/2} \xi_k D_k \varphi_{\Omega,1}^n(\cdot; 0) \text{ and } X_{\Omega,2}^n = |\Omega|^{1/2} \xi_k \xi_l D_{kl}^2 \varphi_{\Omega,1}^n(\cdot; 0).$$

Then, following [7, Proposition 3.2], the fourth order derivative of $\lambda_{\Omega,1}^n(\xi)$ at $\xi = 0$ is defined as

$$\begin{aligned} \frac{1}{4!} D_{klmn}^4 \lambda_{\Omega,1}^n(0) \xi_k \xi_l \xi_m \xi_n &= -\frac{1}{|\Omega|} \int_{\Omega} \mathcal{A}^n \left(X_{\Omega,2}^n - \frac{1}{2} (X_{\Omega,1}^n)^2 \right) \cdot \left(X_{\Omega,2}^n - \frac{1}{2} (X_{\Omega,1}^n)^2 \right) dx \\ &\leq 0. \end{aligned} \tag{3.13}$$

Moreover, using (3.7) and (3.11), the above expression (3.13) becomes

$$\begin{aligned} \frac{1}{4!} D_{klmn}^4 \lambda_{\Omega,1}^n(0) \xi^4 &= -\frac{1}{|\Omega|} \sum_p \varepsilon_{p,n}^{N+2} \int_{\omega} \mathcal{A} \left(X_{\omega}^{(2)} - \frac{1}{2} (X_{\omega}^{(1)})^2 \right) \cdot \left(X_{\omega}^{(2)} - \frac{1}{2} (X_{\omega}^{(1)})^2 \right) dy \\ &= \frac{|\omega|}{|\Omega|} \sum_p \varepsilon_{p,n}^{N+2} \cdot \frac{1}{4!} D_{klmn}^4 \lambda_{\omega,1}(0) \xi^4, \end{aligned} \tag{3.14}$$

where the last equality follows from (2.19).

Remark 3.1. The above equality (3.14) establishes the relation between the fourth order derivatives of $\lambda_{\omega,1}$ and $\lambda_{\Omega,1}$. Remember that the first and second order derivatives of them are equal.

Here we define an approximating dispersion tensor d_{HS}^n for the medium with respect to the highest scale factor κ_n^2 as follows:

$$\frac{1}{4!} D_{klmn}^4 \lambda_{\Omega,1}^n(0) = \kappa_n^2 d_{HS}^n.$$

Then, as $n \rightarrow \infty$, we define the *Burnett coefficient* or the dispersion tensor for the medium as follows:

$$d_{HS} = \limsup_{n \rightarrow \infty} d_{HS}^n = \frac{|\omega|}{|\Omega|} \left(\limsup_{n \rightarrow \infty} \kappa_n^{-2} \sum_p \varepsilon_{p,n}^{N+2} \right) \cdot \frac{1}{4!} D_{klmn}^4 \lambda_{\omega,1}(0). \tag{3.15}$$

The above limit always exists finitely. It can be seen through the following simple estimate:

$$\sum_p \varepsilon_{p,n}^{N+2} \leq \kappa_n^2 \sum_p \varepsilon_{p,n}^N = \kappa_n^2 \frac{|\Omega|}{|\omega|} \quad \text{or} \quad \kappa_n^{-2} \sum_p \varepsilon_{p,n}^{N+2} \text{ is uniformly bounded.}$$

The identity (3.15) reads as d_{HS} is a purely locally defined macro quantity incorporating only various scales associated with the structure. For each n , we have the following approximation:

$$\lambda_{\Omega,1}^n(\xi) = M \xi^2 + \kappa_n^2 d_{HS} \xi^4 + o(\kappa_n^2), \quad \xi \in \Omega'_n.$$

Remark 3.2. Remember that the above expression (3.15) is valid only when A is equivalent to M through the existence of $w_{e_k} \in H_{loc}^1(\mathbb{R}^N)$ satisfying (2.8) and with the existence of $\tilde{w}_{kl} \in H^1(\mathbb{R}^N)$ satisfying (3.12), for each $k, l = 1, \dots, N$. In the next section, as an example of ‘‘Spherical inclusions in two-phase medium’’, we establish their existence.

Remark 3.3. For the periodic micro-structures with the uniform ε -scaling and translation, the above definition (3.15) of the dispersion tensor coincides with the coefficient d_Y defined in (2.4). \square

Motivated by the optimal design and so on, an interesting question that can be taken into account in this matter pertains to which Vitali coverings are responsible for the minimum or maximum value for d_{HS} . In this regard, we prove the conjecture stated below.

Conjecture: *Minimizer of the dispersion tensor is unique among 2-phase periodic Hashin–Shtrikman micro-structures of a given proportion and it is given by the Apollonian–Hashin–Shtrikman micro-structure.*

This conjecture was arrived at by a previous study of the same problem in one-space dimension [9]. Roughly speaking, the result in one dimension says that the value of “ d ” increases when we increase the number of interfaces between the two phases in the micro-structure. At the maximum value of “ d ”, we have a continuum of interfaces and at the minimum value, there is a unique minimizer with a single interface. We prove this in the following section.

4. Spherical Inclusions in 2-Phase Periodic Hashin–Shtrikman Micro-Structures

In the class of periodic spherical Hashin–Shtrikman micro-structures, we consider the unit cell $Y = [0, 1]^N$ in \mathbb{R}^N and identify with \mathbb{R}^N through \mathbb{Z}^N -translation invariance. We first find a Hashin–Shtrikman construction to cover the whole space \mathbb{R}^N and if it is invariant under \mathbb{Z}^N -translations, then we will consider it as a Hashin–Shtrikman structure for Y and conversely. Let us start with a cover for \mathbb{R}^N by a sequence of reduced copy of disjoint balls $B(y^p, \varepsilon_p) = \varepsilon_p B(0, 1) + y^p$ with center y^p and radius ε_p such that

$$meas(\mathbb{R}^N \setminus \bigcup_{p \in \mathbb{K}} B(y^p, \varepsilon_p)) = 0, \text{ where } K \text{ is some infinite countable set}$$

and $m \in \mathbb{Z}^N, \forall p \in K, m + B(y^p, \varepsilon_p) = B(y^p + m, \varepsilon_p) \in \bigcup_{p \in K} B(y^p, \varepsilon_p)$.

Moreover, $\forall m \in \mathbb{Z}^N, meas(\mathbb{R}^N \setminus \bigcup_{p \in \mathbb{K}} (m + B(y^p, \varepsilon_p))) = 0.$ (4.1)

Consequently, the unit periodic cell Y is understood as

$$Y = \bigcup_{p \in K} ([0, 1]^N \cap B(y^p, \varepsilon_p)).$$

Let us now consider $a_B(y)$ to be the two-phase conductivity profile in $B(0, 1)$, defined as follows:

$$a_B(y) = a(r) = \begin{cases} \alpha & \text{if } |y| < R, \\ \beta & \text{if } R < |y| < 1, \end{cases}$$

with $0 < \alpha \leq \beta < \infty$. We define $\theta = R^N$ as the volume proportion of the two-phase profile.

Then $a_B(y)$ is *equivalent* to some m ($\alpha \leq m \leq \beta$) (see [20, page no. 282]), that is, after extending $a_B(y)$ by $a_B(y) = m$ in $\mathbb{R}^N \setminus B(0, 1)$, for each unit vector $e_l \in \mathbb{R}^N$ ($l = 1, \dots, N$), there exists $w_{e_l} \in H^1_{loc}(\mathbb{R}^N)$ satisfying

$$-div(a_B(y)\nabla w_{e_l}(y)) = 0 \text{ in } \mathbb{R}^N, \quad w_{e_l}(y) = y \cdot e_l \text{ in } \mathbb{R}^N \setminus B(0, 1). \tag{4.2}$$

The co-normal flux satisfies

$$a_B(y)\nabla w_{e_l}(y) \cdot \nu = m \text{ on } \partial B(0, 1),$$

where m satisfies the relation

$$\frac{m - \beta}{m + (N - 1)\beta} = \theta \frac{\alpha - \beta}{\alpha + (N - 1)\beta}. \tag{4.3}$$

Now, by homothecy, we extend a_B to the entire \mathbb{R}^N defining

$$a_{\mathbb{R}^N}(y) = a_B\left(\frac{y - y^p}{\varepsilon_p}\right) \text{ in } B(y^p, \varepsilon_p) \text{ almost everywhere in } \mathbb{R}^N$$

and reveal that $a_{\mathbb{R}^N}(y)$ is a Y -periodic function due to (4.1), that is $a_{\mathbb{R}^N} \in L^\infty_\#(Y)$. We define

$$a_Y(y) = a_{\mathbb{R}^N}(y), \quad y \in Y = [0, 1]^N.$$

Next, we set

$$a^\varepsilon(x) = a_Y\left(\frac{x}{\varepsilon}\right), \quad x \in \mathbb{R}^N \text{ and } \frac{x}{\varepsilon} = y \in Y$$

and extend it to the whole \mathbb{R}^N by ε -periodicity with a small period of scale ε , which is considered as two-phase periodic Hashin–Shtrikman micro-structures with spherical inclusions.

(i) *Homogenized coefficients:* The sequence $a^\varepsilon \xrightarrow{H\text{-converges}} m$. One defines $\chi_l \in H^1_\#(Y)$ (see [14, page no. 195]) solving the cell-problem in the periodic cell Y a follows:

$$-div(a_Y(y)(\nabla \chi_l(y) + e_l)) = 0 \text{ in } Y, \quad \text{where } \chi_l \in H^1_\#(Y) \text{ with } \int_Y \chi_l dy = 0. \tag{4.4}$$

Then, one needs to show that the homogenized coefficient a^* , defined below, is equal to m , that is

$$a^* = \frac{1}{|Y|} \int_Y a_Y(y)(\nabla \chi_l(y) + e_l) \cdot (\nabla \chi_l(y) + e_l) dy = m. \tag{4.5}$$

Let us first look for a solution of the following extended equation in the entire space \mathbb{R}^N :

$$-div(a_{\mathbb{R}^N}(y)(\nabla \chi_{\mathbb{R}^N} + e)) = 0 \text{ in } \mathbb{R}^N, \quad \chi_{\mathbb{R}^N} \in H^1_{loc}(\mathbb{R}^N), \tag{4.6}$$

where e is some canonical basis vector in \mathbb{R}^N .

Prior to this, we define

$$\chi_{\mathbb{R}^N}(y) = \varepsilon_p \left(w_e \left(\frac{y - y^p}{\varepsilon_p} \right) - \left(e \cdot \frac{y - y^p}{\varepsilon_p} \right) \right) \text{ if } y \in B(y^p, \varepsilon_p). \tag{4.7}$$

Then, we see that $\chi_{\mathbb{R}^N}$ is a $H^1_{loc}(\mathbb{R}^N)$ -function and it solves the problem (4.6) restricted into each balls $\{B(y^p, \varepsilon_p)\}_{p \in K}$. Moreover, for any $\varphi \in \mathcal{D}(\mathbb{R}^N)$, we have

$$\int_{\mathbb{R}^N} a_{\mathbb{R}^N}(y)(\nabla \chi_{\mathbb{R}^N}(y) + e) \cdot \nabla \varphi(y) \, dy = 0.$$

The above equality follows in a similar manner that we did before for (3.8); it establishes that (4.7) solves (4.6) locally in \mathbb{R}^N .

Now, we claim that, $\chi_{\mathbb{R}^N}(y)$ is a Y -periodic function, that is $\chi_{\mathbb{R}^N} \in H^1_{\#}(Y)$. It simply follows by using (4.1), that is for $y \in \mathbb{R}^N$ and $m \in \mathbb{Z}^N$, we have

$$\begin{aligned} \chi_{\mathbb{R}^N}(y - m) &= \varepsilon_p \left(w_e \left(\frac{y - m - y^p}{\varepsilon_p} \right) - \left(e \cdot \frac{y - m - y^p}{\varepsilon_p} \right) \right) \text{ if } y - m \in B(y^p, \varepsilon_p) \\ &= \varepsilon_p \left(w_e \left(\frac{y - y^{p'}}{\varepsilon_p} \right) - \left(e \cdot \frac{y - y^{p'}}{\varepsilon_p} \right) \right) \text{ if } y \in B(y^{p'}, \varepsilon_p) = B(m + y^p, \varepsilon_p) \\ &= \chi_{\mathbb{R}^N}(y) \text{ (due to (4.1)).} \end{aligned}$$

We define

$$\widetilde{\chi}_Y(y) = \chi_{\mathbb{R}^N}(y), \quad y \in Y = [0, 1]^N.$$

Then $\widetilde{\chi}_Y(y) \in H^1_{\#}(Y)$ and by simply considering $\chi_Y(y) = \widetilde{\chi}_Y(y) - \frac{1}{|Y|} \int_Y \widetilde{\chi}_Y(y) \, dy$, this solves (4.4) for each $e = e_l$. Finally, by taking $\chi_Y(y)$ in the integral identity (4.5) and using (4.2), it follows the homogenized coefficient m . More precisely, we have

$$\begin{aligned} &\frac{1}{|Y|} \int_Y a_Y(y)(\nabla \chi_Y(y) + e) \cdot (\nabla \chi_Y(y) + e) \, dy \\ &= \frac{1}{|Y|} \sum_p \int_{B(y^p, \varepsilon_p) \cap Y} a \left(\frac{y - y^p}{\varepsilon_p} \right) \left| \nabla w_e \left(\frac{y - y^p}{\varepsilon_p} \right) \right|^2 \, dy \\ &= \frac{1}{|B(0, 1)|} \int_{B(0, 1)} a(z) |\nabla w_{e_l}(z)|^2 \, dz = m. \end{aligned}$$

It now remains to establish the relation (4.3). We seek the solution of the above equation (4.2) in the following form:

$$w_{e_l}(y) = y_l f(r), \quad y \in B(0, 1), \tag{4.8}$$

where $f(r)$ is given by

$$f(r) = \begin{cases} \widetilde{b}_1 & \text{if } r < R, \\ \widetilde{b}_2 + \frac{\widetilde{c}}{r^N} & \text{if } R < r < 1, \\ 1 & \text{if } 1 < r. \end{cases} \tag{4.9}$$

In order to keep the solution $w_{e_l}(y)$ and flux $a(r)(f(r) + rf'(r))$ continuous across the inner boundary ($r = R$) and the outer boundary ($r = 1$), we need to impose the following conditions:

$$\begin{aligned} \tilde{b}_1 &= \tilde{b}_2 + \frac{\tilde{c}}{r_1^N}, \quad \alpha \tilde{b}_1 = \beta \left(\tilde{b}_2 + \frac{(1-N)\tilde{c}}{r_1^N} \right), \\ \tilde{b}_2 + \tilde{c} &= 1 \quad \text{and} \quad \beta(\tilde{b}_2 + (1-N)\tilde{c}) = m, \end{aligned} \tag{4.10}$$

Then, solving $(\tilde{b}_1, \tilde{b}_2, \tilde{c})$ in terms of (α, β, θ) from the first three equation of (4.10), we have

$$\tilde{b}_1 = \frac{N\beta}{(1-\theta)\alpha + (N+\theta-1)\beta}, \quad \tilde{b}_2 = \frac{(1-\tilde{b}_1\theta)}{(1-\theta)} \quad \text{and} \quad \tilde{c} = \frac{(\tilde{b}_1-1)\theta}{(1-\theta)} \tag{4.11}$$

and finally putting it into the fourth equation of (4.10), m can be written as in (4.3).

(ii) *Dispersion coefficient:* In the periodic Hashin–Shtrikman structures we denote the dispersion tensor by d_{PHS} . Concerning to our case, we recall the integral expression (2.7) to write d_{PHS} as follows:

$$d_{PHS}\eta^4 = -\frac{1}{|Y|} \int_Y \mathcal{A}_Y \left(X_Y^{(2)} - \frac{(X_Y^{(1)})^2}{2} \right) \cdot \left(X_Y^{(2)} - \frac{(X_Y^{(1)})^2}{2} \right) dy, \tag{4.12}$$

where $\mathcal{A}_Y, X_Y^{(1)}, X_Y^{(2)}$ are defined in (2.5).

Let us denote $X_{B(0,1)}^{(1)}(y) = \eta_k(w_{e_k}(y) - y_k)$, where w_{e_k} is the solution of (4.2) and $X_{B(0,1)}^{(2)} = \eta_k \eta_l w_{kl}$, where w_{kl} is the solution of the following auxiliary cell-equation in $B(0, 1)$:

$$\begin{aligned} -div(a_B(y)\nabla w_{kl}(y)) &= a_B(y)\delta_{kl} - m\delta_{kl} \\ &\quad - \frac{1}{2} \left(C_l^B(w_{e_k}(y) - y_k) + C_k^B(w_{e_l}(y) - y_l) \right) \text{ in } B(0, 1), \\ w_{kl}(y) &= 0 \text{ on } \partial B(0, 1), \end{aligned} \tag{4.13}$$

where $C_k^B(\varphi) = -a_B(y) \frac{\partial \varphi}{\partial x_k} - \frac{\partial}{\partial x_k}(a_B(y)\varphi)$.

We observe that (4.13) is an elliptic partial differential equation with Dirichlet boundary condition which possess an unique solution $w_{kl} \in H_0^1(B(0, 1))$. Having this, we claim that the co-normal derivative of w_{kl} on $\partial B(0, 1)$ is zero, that is

$$\nabla w_{kl}(y) \cdot \nu = 0 \quad \text{on } \partial B(0, 1). \tag{4.14}$$

Remark 4.1. If we extend $a_B(y)$ by m in $\mathbb{R}^N \setminus B(0, 1)$ and $w_{e_k}(y)$ by y_k in $\mathbb{R}^N \setminus B(0, 1)$, then (4.13) becomes

$$-div(m\nabla \widetilde{w}_{kl}(y)) = 0 \quad \text{in } \mathbb{R}^N \setminus B(0, 1) \quad \text{with} \quad \widetilde{w}_{kl}(y) = 0 \text{ on } \partial B(0, 1). \tag{4.15}$$

If $\widetilde{w}_{kl} \in H^1(\mathbb{R}^N \setminus B(0, 1))$, then simply using the maximum principle (see [15, Page no. 164, (3.10)]), we get $\widetilde{w}_{kl}(y) = 0$ in $\mathbb{R}^N \setminus B(0, 1)$, which says that 0 is the natural extension.

Let us define

$$\widetilde{w}_{kl} = \begin{cases} w_{kl} & \text{in } B(0, 1), \\ 0 & \text{in } \mathbb{R}^N \setminus B(0, 1). \end{cases} \tag{4.16}$$

Now, if (4.16) solves both (4.13) and (4.15) as a $H^1(\mathbb{R}^N)$ -function, then from the continuity of the boundary normal flux, we have

$$a_B(y)\nabla w_{kl}(y) \cdot \nu = 0 \quad \text{on } \partial B(0, 1) \quad \text{or} \quad \nabla w_{kl}(y) \cdot \nu = 0 \quad \text{on } \partial B(0, 1).$$

However, at this moment we don't know whether \widetilde{w}_{kl} is a $H^1(\mathbb{R}^N)$ -function or not. Secondly, as we have experienced from the previous case, it is required to have such an extension property in order to get $\chi_{kl} \in H^1_\#(Y)$ from $w_{kl} \in H^1_0(B)$, which solves the cell-problem (2.6).

Proposition 4.1. *The unique solution w_{kl} of (4.13) satisfies the additional boundary condition (4.14).*

Proof. The proof is divided into several steps. We begin with calculating the right hand side of the equation (4.13).

Step 1) RHS of (4.13): Following the definition of the 1st order operator C_l^B and $w_{e_k}(y) = y_k f(r)$, we get

$$\begin{aligned} -C_l^B(w_{e_k}(y) - y_k) &= a(r) \frac{\partial}{\partial y_l}(w_{e_k}(y) - y_k) + \frac{\partial}{\partial y_l}(a(r)(w_{e_k}(y) - y_k)) \\ &= 2a(r)(f(r) - 1)\delta_{kl} + y_k y_l \left(a(r) \frac{f'(r)}{r} + \frac{(a(r)(f(r) - 1))'}{r} \right). \end{aligned}$$

Alternatively,

$$\begin{aligned} a(r)\delta_{kl} - m\delta_{kl} - \frac{1}{2}(C_l^B(w_{e_k}(y) - y_k) + C_k^B(w_{e_l}(y) - y_l)) \\ = a(r)\delta_{kl} - m\delta_{kl} + 2a(r)(f(r) - 1)\delta_{kl} \\ + y_k y_l \left(a(r) \frac{f'(r)}{r} + \frac{(a(r)(f(r) - 1))'}{r} \right). \end{aligned} \tag{4.17}$$

The structure of RHS suggests the following ansatz for the solution of (4.13):

$$w_{kl}(y) = y_k y_l g(r) + h(r).$$

LHS of (4.13): We have

$$\frac{\partial w_{kl}}{\partial y_m}(y) = y_k y_l g'(r) \frac{y_m}{r} + y_k g(r)\delta_{lm} + y_l g(r)\delta_{km} + h'(r) \frac{y_m}{r}.$$

Consequently,

$$\begin{aligned} \frac{\partial}{\partial y_m} \left(a(r) \frac{\partial w_{kl}}{\partial y_m}(y) \right) &= y_k y_l y_m \left(\frac{a(r)g'(r)}{r} \right)' \frac{y_m}{r} + y_k y_l \frac{a(r)g'(r)}{r} \\ &+ y_k \delta_{lm} y_m \frac{a(r)g'(r)}{r} + y_l \delta_{km} y_m \frac{a(r)g'(r)}{r} \\ &+ 2\delta_{km} \delta_{lm} a(r)g(r) + y_k y_m \delta_{lm} \frac{(a(r)g(r))'}{r} \\ &+ y_l y_m \delta_{km} \frac{(a(r)g(r))'}{r} + \frac{a(r)h'(r)}{r} \\ &+ y_m \left(\frac{a(r)h'(r)}{r} \right)' \frac{y_m}{r}, \end{aligned}$$

or

$$\begin{aligned} \text{div}(a(r)\nabla w_{kl}(y)) &= y_k y_l \left(r \left(\frac{a(r)g'(r)}{r} \right)' + (N+2) \frac{a(r)g'(r)}{r} + 2 \frac{(a(r)g(r))'}{r} \right) \\ &+ 2a(r)g(r)\delta_{kl} + N \frac{a(r)h'(r)}{r} + r \left(\frac{a(r)h'(r)}{r} \right)'. \end{aligned} \tag{4.18}$$

Step 2) Both LHS (4.18) and RHS (4.17) contain the quadratic term $y_k y_l$ and the constant term in y . Equating the corresponding coefficients, we get

$$\begin{aligned} r \left(\frac{a(r)g'(r)}{r} \right)' + (N+2) \frac{a(r)g'(r)}{r} + 2 \frac{(a(r)g(r))'}{r} \\ = - \left[a(r) \frac{f'(r)}{r} + \frac{(a(r)(f(r)-1))'}{r} \right] \end{aligned} \tag{4.19}$$

and

$$\begin{aligned} 2a(r)g(r)\delta_{kl} + N \frac{a(r)h'(r)}{r} + r \left(\frac{a(r)h'(r)}{r} \right)' \\ = - \left[a(r)\delta_{kl} - m\delta_{kl} + 2a(r)(f(r)-1)\delta_{kl} \right]. \end{aligned} \tag{4.20}$$

We have

$$a(r) = \alpha \quad \text{and} \quad f(r) = \tilde{b}_1 \quad \text{when } r < R$$

and

$$a(r) = \beta \quad \text{and} \quad f(r) = \tilde{b}_2 + \frac{\tilde{c}}{r^N} \quad \text{when } R < r < 1,$$

where $(\tilde{b}_1, \tilde{b}_2, \tilde{c})$ are known in terms of α, β, N and θ (see (4.11)).

We further seek $h(r)$ and $g(r)$ in the general form of

$$g(r) = b + \frac{c}{r^N} + \frac{d}{r^{N+2}} \quad \text{and} \quad h(r) = \left(\frac{p}{r^N} + qr^2 + t \right) \delta_{kl}. \tag{4.21}$$

The set of constants (b, c, d) and (p, q, t) can take different values in the ranges $r < R$ and $R < r < 1$. We denote them by (b_1, c_1, d_1) , (p_1, q_1, t_1) and (b_2, c_2, d_2) , (p_2, q_2, t_2) , respectively.

Now, by using (4.21) in (4.19), we get the following cases:

Case 1. When $r < R$, we have

$$-N(N + 2)\frac{c_1}{r^{N+2}} - (N + 2)^2\frac{d_1}{r^{N+4}} + N(N + 2)\frac{c_1}{r^{N+2}} + (N + 4)(N + 2)\frac{d_1}{r^{N+4}} + 2\left(-N\frac{c_1}{r^{N+2}} - (N + 2)\frac{d_1}{r^{N+4}}\right) = 0,$$

or

$$\frac{c_1}{r^{N+2}}(-N(N + 2) + N(N + 2) - 2N) + \frac{d_1}{r^{N+4}}(-N(N + 2)^2 + (N + 4)(N + 2) - 2(N + 2)) = 0,$$

or

$$-2N\frac{c_1}{r^{N+2}} = 0,$$

which implies $c_1 = 0$.

Case 2. When $R < r < 1$, we have

$$-2N\frac{c_2}{r^{N+2}} = -2N\frac{\tilde{c}}{r^{N+2}},$$

which implies $c_2 = -\tilde{c}$.

Moreover, using (4.21) in (4.20), we get

Case 1. When $r < R$, we have

$$\alpha\left[2\left(b_1 + \frac{d_1}{r^{N+2}}\right)\delta_{kl} - N^2\frac{p_1}{r^{N+2}} + N(N + 2)\frac{p_1}{r^{N+2}} + 2Nq_1\right] = -[\alpha - m + 2\alpha(\tilde{b}_1 - 1)]\delta_{kl},$$

or

$$\alpha(2d_1\delta_{kl} - N^2p_1 + N(N + 2)p_1)\frac{1}{r^{N+2}} + \alpha(2b_1\delta_{kl} + 2Nq_1) = -[\alpha - m + 2\alpha(\tilde{b}_1 - 1)]\delta_{kl},$$

which implies that

$$d_1\delta_{kl} + Np_1 = 0 \tag{4.22}$$

$$\text{and } \alpha(2b_1\delta_{kl} + 2Nq_1) = -[\alpha - m + 2\alpha(\tilde{b}_1 - 1)]\delta_{kl}. \tag{4.23}$$

Case 2. When $R < r < 1$, we have

$$\beta\left[2\left(b_2 + \frac{c_2}{r^N} + \frac{d_2}{r^{N+2}}\right)\delta_{kl} + 2N\frac{p_2}{r^{N+2}} + 2Nq_2\right] = -\left[\beta - m + 2\beta(\tilde{b}_2 - 1 + \frac{\tilde{c}}{r^N})\right]\delta_{kl},$$

then, by using $c_2 = -\tilde{c}$, it gives

$$d_2\delta_{kl} + Np_2 = 0 \tag{4.24}$$

$$\text{and } \beta(2b_2\delta_{kl} + 2Nq_2) = -[\beta - m + 2\beta(\tilde{b}_2 - 1)]\delta_{kl}. \tag{4.25}$$

Step 3) Boundary Conditions:

i) Transmission conditions:

a) Continuity of the w_{kl} over the inner boundary at $r = R$:

$$b_1 + \frac{d_1}{R^{N+2}} = b_2 + \frac{-\tilde{c}}{R^N} + \frac{d_2}{R^{N+2}}, \tag{4.26}$$

$$\left(\frac{p_1}{R^N} + q_1R^2 + t_1\right)\delta_{kl} = \left(\frac{p_2}{R^N} + q_2R^2 + t_2\right)\delta_{kl}. \tag{4.27}$$

b) Continuity of the flux over the inner boundary at $r = R$: We must rewrite the equation (4.13) in the following divergence form of

$$\begin{aligned} -\frac{\partial}{\partial y_m} a(r) \left(\frac{\partial}{\partial y_m} w_{kl}(y) + \frac{1}{2}((w_{ek}(y) - y_k)\delta_{lm} + (w_{el}(y) - y_l)\delta_{km}) \right) \\ = a(r)\delta_{kl} - m\delta_{kl} + \frac{1}{2}a(r) \left(\frac{\partial}{\partial y_k} (w_{el}(y) - y_l) + \frac{\partial}{\partial y_l} (w_{ek}(y) - y_k) \right). \end{aligned}$$

Thus, the boundary normal flux term, which we are concerned with, becomes

$$\begin{aligned} a(r) \left(\frac{\partial}{\partial y_m} (w_{kl}(y)) + \frac{1}{2}((w_{ek}(y) - y_k)\delta_{km} + (w_{el}(y) - y_l)\delta_{km}) \right) \cdot \nu \\ = a(r) \left(\frac{\partial}{\partial y_m} (y_k y_l g(r) + h(r)) + \frac{1}{2}(y_k(f(r) - 1)\delta_{km} + y_l(f(r) - 1)\delta_{km}) \right) \frac{y_m}{r} \\ = y_k y_l \left(a(r) \left(g'(r) + 2\frac{g(r)}{r} + \frac{f(r) - 1}{r} \right) \right) + a(r)h'(r). \end{aligned}$$

Thus, from the required continuity of the boundary normal flux over the inner boundary at $r = R$, we get

$$\begin{aligned} \alpha \left[\left(b_1 + \frac{d_1}{r^{N+2}} \right)' + 2\frac{\left(b_1 + \frac{d_1}{r^{N+2}} \right)}{r} + \frac{(\tilde{b}_1 - 1)}{r} \right] \Big|_{r=R} \\ = \beta \left[\left(b_2 + \frac{-\tilde{c}}{r^N} + \frac{d_2}{r^{N+2}} \right)' + 2\frac{b_2 + \frac{-\tilde{c}}{r^N} + \frac{d_2}{r^{N+2}}}{r} + \frac{\tilde{b}_2 + \frac{-\tilde{c}r^N - 1}{r}}{r} \right] \Big|_{r=R} \end{aligned} \tag{4.28}$$

and

$$\alpha \left(\frac{p_1}{r^N} + q_1r^2 + t_1 \right)' \Big|_{r=R} \delta_{kl} = \beta \left(\frac{p_2}{r^N} + q_2r^2 + t_2 \right)' \Big|_{r=R} \delta_{kl}. \tag{4.29}$$

ii) Dirichlet boundary condition: From the Dirichlet boundary condition of w_{kl} on $\partial B(0, 1)$, we get

$$b_2 - \tilde{c} + d_2 = 0, \tag{4.30}$$

$$(p_2 + q_2 + t_2)\delta_{kl} = 0. \tag{4.31}$$

Step 4) The unknown constants $(b_1, d_1), (p_1, q_1, r_1)$ and $(b_2, d_2), (p_2, q_2, t_2)$ can be found uniquely by solving equations (4.22) to (4.31). There are 10 unknown constants, 10 linearly independent equations. Here, 10 coefficients are uniquely determined, this confirms the already known fact, namely, unique solution to (4.13). Now, we claim that the co-normal derivative of w_{kl} on $\partial B(0, 1)$ is zero, that is

$$\nabla w_{kl}(y) \cdot \nu = 0 \quad \text{on } \partial B(0, 1). \tag{4.32}$$

The above equation, (4.14), is equivalent to two linear equations involving the coefficients (b_2, d_2) and (p_2, q_2, t_2) as follows:

$$\left[(b_2 + \frac{-\tilde{c}}{r^N} + \frac{d_2}{r^{N+2}})' + 2 \frac{b_2 + \frac{-\tilde{c}}{r^N} + \frac{d_2}{r^{N+2}}}{r} \right] |_{r=1} = 0 \tag{4.33}$$

and
$$\left(\frac{p_2}{r^N} + q_2 r^2 + t_2 \right)' |_{r=1} \delta_{kl} = 0. \tag{4.34}$$

In order to establish our claim we have to show with the addition of these two new linear equations (4.33), (4.34), that all of these 12 linear equations (4.22) to (4.34) form a consistent system of 10 unknown coefficients. To this end, (for case of computation), we replace (4.25) and (4.29) by (4.33) and (4.34), and we solve the resulting system of 10 equations; their solution is then shown to satisfy (4.25), (4.29) as well.

First, we determine d_2 from (4.33) and consequently p_2 and q_2 from (4.24) and (4.34), respectively, to get

$$(N + 2)d_2 - N\tilde{c} = 0, \quad \text{or } d_2 = \frac{N}{(N + 2)}\tilde{c}, \tag{4.35}$$

$$d_2\delta_{kl} + Np_2 = 0, \quad \text{or } p_2 = -\frac{1}{(N + 2)}\tilde{c} \delta_{kl}, \tag{4.36}$$

$$(-Np_2 + 2q_2) = 0, \quad \text{or } q_2 = -\frac{N}{2(N + 2)}\tilde{c} \delta_{kl}. \tag{4.37}$$

Then, we determine b_2 and t_2 from (4.30) and (4.31), respectively, to get

$$b_2 = \frac{2}{(N + 2)}\tilde{c}, \quad t_2 = \frac{1}{2}\tilde{c} \delta_{kl}. \tag{4.38}$$

Next, we consider (4.26) and (4.28) to determine (b_1, d_1) and we get

$$\begin{aligned} \alpha(N + 2)b_1 &= (\beta(\tilde{b}_2 + \frac{\tilde{c}}{R^N} - 1) - \alpha(\tilde{b}_1 - 1)) \\ &+ \alpha\left(\frac{2}{(N + 2)} - \frac{1}{R^N} + \frac{N}{(N + 2)}\frac{1}{R^{N+2}}\right)\tilde{c} \\ &+ \beta\left(\frac{4}{(N + 2)} + \frac{(N - 2)}{R^N} - \frac{N^2}{(N + 2)}\frac{1}{R^{N+2}}\right)\tilde{c} \end{aligned}$$

and

$$\begin{aligned} \alpha(N+2)\frac{d_1}{R^{N+2}} &= -(\beta(\tilde{b}_2 + \frac{\tilde{c}}{R^N} - 1) - \alpha(\tilde{b}_1 - 1)) \\ &+ 2\alpha\left(\frac{2}{(N+2)} - \frac{1}{R^N} + \frac{N}{(N+2)}\frac{1}{R^{N+2}}\right)\tilde{c} \\ &- \beta\left(\frac{4}{(N+2)} + \frac{(N-2)}{R^N} - \frac{N^2}{(N+2)}\frac{1}{R^{N+2}}\right)\tilde{c}. \end{aligned}$$

Successively, we can find p_1, q_1 and t_1 from (4.22), (4.23) and (4.27), respectively.

Thus we have determined all 10 coefficients and it is remained to check that the solutions obtained above satisfies (4.25) and (4.29). We recall (4.11) to write

$$\begin{aligned} \tilde{b}_2 - 1 &= -\tilde{c} \quad \text{and} \quad \tilde{b}_1 - 1 = \frac{(1-\theta)}{\theta}\tilde{c}, \quad \text{where } \theta = R^N, \\ m - \beta &= -N\beta\tilde{c} \quad \text{and} \quad m - \alpha = \frac{(1-\theta)((N-1)\beta + \alpha)}{\theta}\tilde{c}. \end{aligned}$$

Now, let us see that the LHS of (4.25) is equal to

$$\beta(2b_2\delta_{kl} + 2Nq_2) = \beta\left(2\frac{2}{(N+2)}\tilde{c}\delta_{kl} - 2N\frac{N}{2(N+2)}\tilde{c}\right) = \beta(2-N)\tilde{c}\delta_{kl}$$

and the RHS of (4.25) is equal to

$$-(\beta - m)\delta_{kl} - 2\beta(\tilde{b}_2 - 1)\delta_{kl} = -N\beta\tilde{c}\delta_{kl} + 2\beta\tilde{c}\delta_{kl} = \beta(2-N)\tilde{c}\delta_{kl},$$

which is exactly equal to the LHS of (4.25).

Next, we consider (4.29) and we have that

$$\begin{aligned} \text{LHS of (4.29)} &:= \alpha\left(\frac{p_1}{r^N} + q_1r^2 + t_1\right)' \Big|_{r=R} \delta_{kl} = \alpha\left(-\frac{Np_1}{R^{N+1}} + 2q_1R\right) \\ &= R\alpha\left(\frac{d_1}{R^{N+2}} + 2q_1\right) \\ &= R\left(\alpha\frac{d_1}{R^{N+2}} + \frac{-2\alpha b_1 - (\alpha - m) - 2\alpha(\tilde{b}_1 - 1)}{N}\delta_{kl}\right) \\ &= R\beta\frac{N}{N+2}\left(\frac{1}{R^{N+2}} - 1\right)\tilde{c}. \\ \text{RHS of (4.29)} &:= \beta\left(\frac{p_2}{r^N} + q_2r^2 + t_2\right)' \Big|_{r=R} = \beta\left(-\frac{Np_2}{R^{N+1}} + 2q_2R\right) \\ &= R\beta\frac{N}{N+2}\left(\frac{1}{R^{N+2}} - 1\right)\tilde{c} \\ &= \text{LHS of (4.29)}. \end{aligned}$$

Therefore, all 12 of these linear equations (4.22) to (4.29) form a consistent system for 10 variables and which establishes our claim of having zero Neumann data together with zero Dirichlet data on the boundary of the unit ball. \square

Resolution of (2.5): Then, as we did before (see (4.7)), using $w_{kl} \in H_0^1(B(0, 1))$ with $\nabla w_{kl} \cdot \nu = 0$ on $\partial B(0, 1)$, we will define $\chi_{kl} \in H_{\#}^1(Y)$ in order to solve (2.5). First, we define $\widetilde{\chi}_{kl} \in H_{loc}^1(\mathbb{R}^N)$ by

$$\widetilde{\chi}_{kl}(y) = \varepsilon_p^2 w_{kl}\left(\frac{y - y^p}{\varepsilon_p}\right) \text{ in } B(y^p, \varepsilon_p) \text{ almost everywhere in } \mathbb{R}^N,$$

solving

$$-div(a_{\mathbb{R}^N}(y)\nabla\widetilde{\chi}_{kl}(y)) = a_{\mathbb{R}^N}(y)\delta_{kl} - m\delta_{kl} - \frac{1}{2}(C_l(\chi_k) + C_k(\chi_l)) \text{ in } \mathbb{R}^N. \tag{4.39}$$

Then, we conclude that $\widetilde{\chi}_{kl}$ is a Y -periodic function and in order to get $\chi_{kl} \in H_{\#}^1(Y)$ with $\int_Y \chi_{kl} dy = 0$ solving (4.39) in Y , we simply define $\chi_{kl}(y) = \widetilde{\chi}_{kl}(y) - \frac{1}{|Y|} \int_Y \widetilde{\chi}_{kl} dy$, by restricting it in Y . Subsequently, one has $X_Y^{(2)} = \eta_k \eta_l \chi_{kl}$, which solves the cell-problem (2.5).

Expression for d_{PHS} : Hence, the integral identity (4.12) of d_{PHS} becomes

$$\begin{aligned} -|Y| \cdot d_{PHS} \eta^4 &= \int_Y \mathcal{A}_Y\left(X_Y^{(2)} - \frac{(X_Y^{(1)})^2}{2}\right) \cdot \left(X_Y^{(2)} - \frac{(X_Y^{(1)})^2}{2}\right) dy \\ &= \sum_p \varepsilon_p^{N+2} \cdot \int_{B(0,1)} \mathcal{A}_{B(0,1)}\left(X_{B(0,1)}^{(2)} - \frac{(X_{B(0,1)}^{(1)})^2}{2}\right) \cdot \left(X_{B(0,1)}^{(2)} - \frac{(X_{B(0,1)}^{(1)})^2}{2}\right) dy. \end{aligned}$$

Elimination of $X_{B(0,1)}^{(2)}$: We simplify the above expression to express it as depending solely on $X_{B(0,1)}^{(1)}$ by eliminating $X_{B(0,1)}^{(2)}$. Let us define $\widetilde{X}_{B(0,1)} = X_{B(0,1)}^{(2)} - \frac{(X_{B(0,1)}^{(1)})^2}{2}$, then using (4.8) and (4.13), we write

$$-div(a_B(y)\nabla\widetilde{X}_{B(0,1)}(y)) = div\left(a_B(y)\nabla\frac{(X_{B(0,1)}^{(1)}(y) + \eta \cdot y)^2}{2}\right) - \widetilde{m} \text{ in } B. \tag{4.40}$$

It simply follows that

$$\begin{aligned} div\left(a_B(y)\nabla\frac{(w_{e_k})^2}{2}\right) &= div\left(a_B(y)\nabla(w_{e_k} - y_k)\right) \cdot (w_{e_k} - y_k) \\ &\quad + a_B(y)\nabla(w_{e_k} - y_k) \cdot \nabla(w_{e_k} - y_k) \\ &= -div(a_B(y)e_k) \cdot (w_{e_k} - y_k) + a_B(y)\nabla(w_{e_k} - y_k) \cdot \nabla(w_{e_k} - y_k) \\ &= a_B(y)(\nabla(w_{e_k} - y_k) + e_k) \cdot (\nabla(w_{e_k} - y_k) + e_k) - a_B(y) + C_k^B(w_{e_k} - y_k) \\ &= div\left(a_B(y)\nabla\frac{((w_{e_k} - y_k) + y_k)^2}{2}\right) - a_B(y) + C_k^B(w_{e_k} - y_k). \end{aligned}$$

Now, multiplying (4.40) by $\widetilde{X}_{B(0,1)}$, doing integration by parts and using the fact that $X_{B(0,1)}^{(1)} = X_{B(0,1)}^{(2)} = 0$ on $\partial B(0, 1)$, we get

$$|Y| \cdot d_{PHS} \eta^4 = \sum_p \varepsilon_p^{N+2} \left[\int_{B(0,1)} a_B(y) \nabla \frac{(X_{B(0,1)}^{(1)} + \eta \cdot y)^2}{2} \cdot \nabla \left(X_{B(0,1)}^{(2)} - \frac{(X_{B(0,1)}^{(1)})^2}{2} \right) - \tilde{m} \int_{B(0,1)} \frac{(X_{B(0,1)}^{(1)})^2}{2} dy \right].$$

Then, multiplying (4.40) by $\frac{(X_{B(0,1)}^{(1)} + \eta \cdot y)^2}{2}$, doing the integration by parts and using the fact that $X_{B(0,1)}^{(1)} = 0$ and $\nabla X_{B(0,1)}^{(2)} \cdot \nu = 0$ on $\partial B(0, 1)$, we finally get

$$-d_{PHS} \eta^4 \cdot |Y| = \sum_p \varepsilon_p^{N+2} \left[\int_{B(0,1)} a_B(y) \nabla \frac{(X_{B(0,1)}^{(1)} + \eta \cdot y)^2}{2} \cdot \nabla \frac{(X_{B(0,1)}^{(1)} + \eta \cdot y)^2}{2} dy + \tilde{m} \int_{B(0,1)} \frac{(X_{B(0,1)}^{(1)})^2}{2} dy \right]. \tag{4.41}$$

Final expression for d_{PHS} : Moreover, due to the explicit formula of the solution $X_{B(0,1)}^{(1)} = \eta_k (w_{e_k}(y) - y_k)$ (see (4.9)) and taking $\eta = e_k$, we express (4.41) as follows:

$$-2|Y| \cdot d_{PHS} = \sum_p \varepsilon_p^{N+2} \cdot \left[\int_{B(0,R)} \tilde{b}_1^2 (m - \alpha \tilde{b}_1^2) y_k^2 dy + \int_{B(0,1) \setminus B(0,R)} \left(m - \beta \left(\tilde{b}_2 + \frac{\tilde{c}}{r^N} \right)^2 \left| \nabla \left(y_k \left(\tilde{b}_2 + \frac{\tilde{c}}{r^N} \right) \right) \right|^2 \right) y_k^2 dy \right], \tag{4.42}$$

where $\tilde{b}_1, \tilde{b}_2, \tilde{c}$ are known in terms of given data α, β, θ and N found in (4.11).

Remark 4.2. It is already known from the expression (4.12) (or (4.41)) that the dispersion tensor d_{PHS} is a non-positive definite tensor. Moreover, the expression (4.41) tells us that d_{PHS} depends upon only on the scales $\{\varepsilon_p\}_{p \in K}$, not on the translations $\{y^p\}_{p \in K}$. The last aspect signifies the following property of d_{PHS} : the position of balls in a micro-structure is not important; what matters is only their radii. Thus, two Hashin–Shtrikman micro-structures consisting of different arrangements of core-coating balls, but having the same set of radii, have the same value of the Bloch dispersion coefficient d_{PHS} . This aspect of Hashin–Shtrikman micro-structure is not obvious to start with. Thus, even though d_{PHS} varies among Hashin–Shtrikman structures, its variation is somewhat special: it does not depend on the position of the centers of balls in the micro-structure; it depends only on the radii. Recall that the homogenized coefficient m depends only on $\{\alpha, \beta, \theta, N\}$, but it is independent of radii $\{\varepsilon_p\}_{p \in K}$ and centers $\{y^p\}_{p \in K}$.

The above computation reduced the original problem which was posed on micro-structures, to the space of sequences l^1 (cf. ‘Conjecture’ at the end of the Section 3). As long as the macro quantities $(\tilde{b}_1, \tilde{b}_2, \tilde{c})$ are getting fixed through (4.11), from the expression (4.42) we can compute d_{PHS} explicitly and moreover, due to the negativity of the dispersion tensor, it will be maximized or minimized whenever $\sum_p \varepsilon_p^{N+2}$ is minimized or maximized, respectively, under the constraint $\sum_p \varepsilon_p^N = c_N$ (a dimension constant). As a next step, we exploit the properties of l^1 to prove the existence of minimizers.

5. Proof of the Conjecture

Let us consider a Vitali covering of $Y = [0, 1]^N$ with a countable infinite union of disjoint balls with center y^p and radius ε_p , where $p \in K$, that is

$$\text{meas}(Y \setminus \bigcup_{p \in K} (B(y^p, \varepsilon_p) \cap Y)) = 0.$$

We first rearrange the sequence $\{\varepsilon_p\}_{p \in K}$ to make it as a decreasing sequence, that is, $\varepsilon_1 \geq \varepsilon_2 \geq \dots \geq \varepsilon_p \geq \dots$. Let us define $d_p = \frac{\varepsilon_p^N}{c_N^N}$, with $d_1 \geq d_2 \geq \dots \geq d_p \geq \dots$. Then, we want to minimize $I = -c_N^{\frac{N+2}{N}} \sum_p d_p^{\frac{N+2}{N}}$ under the constraint $\sum_p d_p = 1$ as follows:

$$\text{Minimization of } I = -c_N^{\frac{N+2}{N}} \sum_p d_p^{\frac{N+2}{N}} \text{ under the constraint } \sum_p d_p = 1.$$

Difficulties with the minimization problem:

The peculiarity of our problem is that it is concerned with a (constrained) minimization of a strictly concave functional over the unit sphere of l^1 (the unit sphere representing the constraint set). From the point of view of Functional Analysis, difficulties with the existence of a minimizer are well-known, owing to the non-reflexivity of l^1 . In general, working in such spaces, a bounded sequence may not have any weakly converging subsequence and even if it has one, we cannot conclude that it satisfies the constraint.

Existence of Minimizers:

Fortunately, in our case, the criterion of de la Vallee-Poussin [16, Page no. 19] is applicable and it guarantees l^1 -weak compactness of a minimizing sequence. It is also known that weak and norm convergences are equivalent in the case of l^1 . These arguments establish that any minimizing sequence has a converging subsequence in l^1 , and so a minimizer satisfying the constraint exists.

Uniqueness Issue:

However, uniqueness is an issue since we have a strictly concave functional to minimize. Uniqueness of the minimizer can however be proved using other arguments, outlined below. Combining both results, we obtain that the entire minimizing sequence is l^1 strongly convergent. It is not clear how uniqueness can be proved by an analytical method. However, with a geometric point of view, we can settle both the existence and the uniqueness of minimizer. This is done in the sequel.

Existence and Uniqueness via Geometrical Method: For a geometrical picture, we ask the reader to imagine the flat torus obtained by identifying the opposite sides of the cell $Y = [0, 1]^N$. We have already seen that the dispersion coefficient d_{PHS} is invariant under translation, and that Y is identified with \mathbb{R}^N through \mathbb{Z}^N -translation invariance. Then, we first find a Hashin–Shtrikman construction to cover the whole space \mathbb{R}^N and if it is invariant under \mathbb{Z}^N -translations, then we will consider it as a Hashin–Shtrikman structure for Y and conversely. Note that it is enough to consider decreasing sequences of non-negative numbers in the minimization process. These numbers represent the radii of balls in the Hashin–Shtrikman micro-structure. Finding the first and highest element of the minimizer

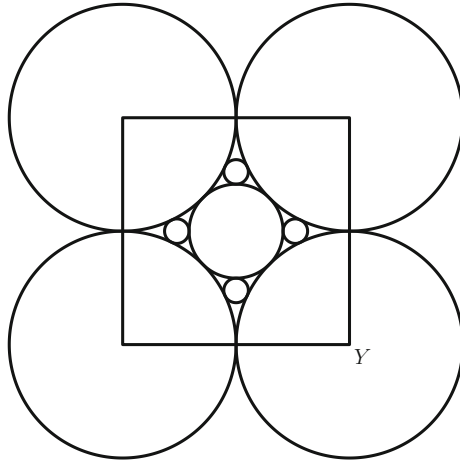


Fig. 2. Apollonian-Hashin-Shtrikman structures in Y .

amounts to putting a ball with maximum radius ($\varepsilon_1^* = \frac{1}{2}$) inside the torus. It is geometrically clear that this ball (and hence its radius) is uniquely determined. In the second step, the same pattern is repeated: the second and next highest element of the minimizer represents the radius ($\varepsilon_2^* = \frac{\sqrt{2}-1}{2}$) of the biggest ball embedded in the complement of the previous ball. Again, this is unique. In the third step, we observe that there is no uniqueness and in fact there are four balls of maximum radii ($\varepsilon_3^* = \frac{(\sqrt{2}-1)(2\sqrt{2}-1)}{14}$), which can be placed in the complement of the union of the first and the second balls. The radii of these four balls are however equal. This amounts to saying that the third, fourth, fifth and sixth elements of the minimizer are equal. The above argument can be repeated at every subsequent step and this procedure identifies the *Apollonian-Hashin-Shtrikman* micro-structures (Figure 2) as the unique solution of our geometric problem. The radii $\{\varepsilon_p^*\}_{p \in K}$ of the balls thus obtained provide the minimizer for our constrained minimization problem. Hence, we denote the minimum value as $I_{min} = -c_N \sum_p^{\frac{N+2}{N}} (\varepsilon_p^*)^{N+2}$.

Optimal bounds on I : We have found the minimum value of I with its unique minimizer; next we find its maximum value under the constraint $\sum_p d_p = 1$. We simply see that

$$I = -c_N \sum_p^{\frac{N+2}{N}} d_p^{\frac{N+2}{N}} \leq -c_N d_1^{\frac{2}{N}}.$$

Clearly, $d_1 > 0$ can be chosen arbitrarily small. Thus, 0 is the supremum value of I and it is not the maximum value of I . Thus, unlike in the previous case of minimization, here the maximizer doesn't exist in the classical micro-structures. In particular, we have a bound for I , that is, $I \in [I_{min}, 0)$. □

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