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Partial differential equations/Numerical analysis

An embedded corrector problem to approximate the homogenized coefficients of an elliptic equation [☆]



Un problème d'inclusion pour approcher les coefficients homogénéisés d'une équation elliptique

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ARTICLE INFO

Article history:

Received 19 December 2014

Accepted after revision 22 June 2015

Available online 4 August 2015

Presented by Olivier Pironneau

ABSTRACT

We consider a diffusion equation with highly oscillatory coefficients that admits a homogenized limit. As an alternative to standard corrector problems, we introduce here an embedded corrector problem, written as a diffusion equation in the whole space, in which the diffusion matrix is uniform outside some ball of radius R . Using that problem, we next introduce three approximations of the homogenized coefficients. These approximations, which are variants of the standard approximations obtained using truncated (supercell) corrector problems, are shown to converge to the homogenized coefficient when $R \rightarrow \infty$. We also discuss efficient numerical methods to solve the embedded corrector problem.

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R É S U M É

Nous considérons une équation de diffusion à coefficients hautement oscillants qui admet une limite homogénéisée, et nous introduisons une variante du problème du correcteur standard, qui se formalise comme un problème d'inclusion. Celui-ci s'écrit comme une équation de diffusion posée dans tout l'espace, dans laquelle la matrice de diffusion est uniforme à l'extérieur d'une boule de rayon R . Nous introduisons ensuite trois approximations des coefficients homogénéisés, calculées à partir de la solution de ce problème. Ces approximations, qui sont des variantes des approximations standard basées sur le problème du correcteur tronqué (méthode de supercellule), convergent lorsque $R \rightarrow \infty$ vers le coefficient homogénéisé. Nous mentionnons également des méthodes de résolution numérique efficaces pour ce nouveau problème.

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[☆] We thank Paul Cazeaux for fruitful discussions on questions related to this project. The work of FL is partially supported by ONR under Grant N00014-12-1-0383 and EOARD under Grant FA8655-13-1-3061.

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<http://dx.doi.org/10.1016/j.crma.2015.06.019>

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1. Introduction

We consider the standard elliptic, highly oscillatory problem

$$-\operatorname{div}[\mathbb{A}(\cdot/\varepsilon) \nabla u_\varepsilon] = f \text{ in } \Omega, \quad u_\varepsilon = 0 \text{ on } \partial\Omega, \tag{1}$$

where Ω is a smooth bounded domain of \mathbb{R}^d and $f \in L^2(\Omega)$. The coefficient \mathbb{A} is a matrix-valued field, and ε is a small characteristic length scale. Throughout this Note, we assume that \mathbb{A} is symmetric and elliptic, in the sense that there exists $0 < \alpha \leq \beta < \infty$ such that $\mathbb{A}(x) \in \mathcal{M}_{\alpha,\beta}$ for any $x \in \mathbb{R}^d$, where

$$\mathcal{M}_{\alpha,\beta} := \left\{ A \in \mathbb{R}^{d \times d}, A^T = A \text{ and, for any } \xi \in \mathbb{R}^d, \alpha |\xi|^2 \leq \xi^T A \xi \leq \beta |\xi|^2 \right\}.$$

It is well known (see, e.g., [2,8,12]) that, under this assumption, problem (1) admits a homogenized limit, i.e. that the sequence $\mathbb{A}(\cdot/\varepsilon)$ G -converges, up to the extraction of a subsequence, to some homogenized matrix-valued field $A^* \in L^\infty(\Omega, \mathcal{M}_{\alpha,\beta})$ when $\varepsilon \rightarrow 0$ (the notion of G -convergence is recalled in Definition 3.1 below).

Our setting includes in particular the periodic case, where $\mathbb{A}(x) = \mathbb{A}_{\text{per}}(x)$ for a fixed \mathbb{Z}^d -periodic function \mathbb{A}_{per} , and the random stationary case (see [13,17]), where

$$\mathbb{A}(x) = \mathbb{A}_{\text{sta}}(x, \omega) \text{ for some realization } \omega \text{ of a random stationary function } \mathbb{A}_{\text{sta}}. \tag{2}$$

In these two cases, the whole sequence $\mathbb{A}(\cdot/\varepsilon)$ G -converges (for almost all ω in the case (2)).

Computing the homogenized coefficient A^* is in general a challenging task, even in the cases when a closed form formula for A^* is available. To motivate our work, consider for instance the random stationary case (2) in a discrete stationary setting [1,3] when

$$\forall k \in \mathbb{Z}^d, \quad \mathbb{A}_{\text{sta}}(x, \tau_k \omega) = \mathbb{A}_{\text{sta}}(x + k, \omega) \quad \text{a.e. in } x, \text{ a.s. in } \omega,$$

where $(\tau_k)_{k \in \mathbb{Z}^d}$ is an ergodic group action on the probability space. In that setting, A^* is a constant deterministic matrix, given by

$$\forall p \in \mathbb{R}^d, \quad A^* p = \mathbb{E} \left[\frac{1}{|Q|} \int_Q \mathbb{A}(x, \cdot) (p + \nabla w_p(x, \cdot)) \, dx \right], \quad Q = (0, 1)^d, \tag{3}$$

where w_p is the unique solution (up to an additive constant) to the so-called corrector problem

$$\begin{cases} -\operatorname{div}[\mathbb{A}(\cdot, \omega)(p + \nabla w_p(\cdot, \omega))] = 0 \text{ almost surely in } \mathcal{D}'(\mathbb{R}^d), \\ \nabla w_p \text{ is stationary, } \quad \mathbb{E} \left[\int_Q \nabla w_p(x, \cdot) \, dx \right] = 0. \end{cases} \tag{4}$$

The major difficulty to compute A^* is the fact that the corrector problem (4) is set over the whole space \mathbb{R}^d and cannot be reduced to a problem posed over a bounded domain (in contrast to, e.g., periodic homogenization). This is the reason why approximation strategies are required, yielding practical approximations of A^* . A popular approach, introduced in [4], is to approximate A^* by $A_N^*(\omega)$, which, in turn, is defined by

$$\forall p \in \mathbb{R}^d, \quad A_N^*(\omega) p := \frac{1}{|Q_N|} \int_{Q_N} \mathbb{A}(x, \omega) (p + \nabla w_p^N(x, \omega)) \, dx, \quad Q_N = (-N, N)^d, \tag{5}$$

where w_p^N is the unique solution (up to an additive constant) to the truncated corrector problem

$$-\operatorname{div}[\mathbb{A}(\cdot, \omega)(p + \nabla w_p^N(\cdot, \omega))] = 0 \text{ almost surely in } \mathcal{D}'(\mathbb{R}^d), \quad w_p^N(\cdot, \omega) \text{ is } Q_N\text{-periodic.} \tag{6}$$

As shown in [4], $A_N^*(\omega)$ almost surely converges to A^* when $N \rightarrow \infty$.

As we have just pointed out, computing the homogenized coefficient A^* is in general a challenging task (we have taken above the example of the stationary setting, but the same conclusion holds for other settings, including, e.g., the quasiperiodic setting). The aim of this Note is to introduce variants of classical formulas (i.e. (5)–(6) in the stationary setting) that allow us to compute accurate approximations of the homogenized coefficient A^* , and that, in some cases, are amenable to efficient numerical implementations through the use of boundary integral formulations. We refer to [14] for other characterizations of the homogenized matrix, which can also be turned into numerical strategies that are an alternative to (5)–(6) to approximate A^* in the random stationary setting. See also [9,11] for other numerical strategies to approximate (3).

In Section 2, we describe our approach and explain in what sense it is amenable to an efficient implementation. Based on that approach, alternative approximations of A^* are built in Section 3, where we also collect convergence results. The results presented in this Note will be complemented and extended in [5].

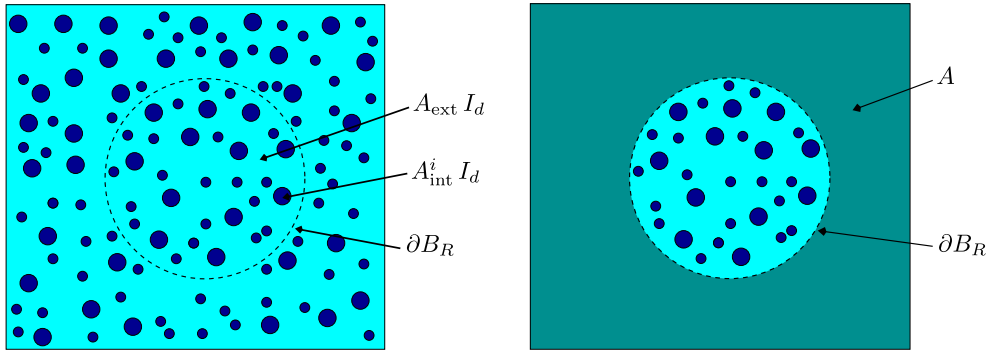


Fig. 1. (Color online.) Left: field $\mathbb{A}(x)$. Right: field $\mathbb{A}_{R,A}(x)$: beyond the sphere of radius R , the field $\mathbb{A}(x)$ is replaced by a uniform coefficient A .

2. Embedded corrector problem

In this section, we introduce an embedded corrector problem (see (7) below), which is key to our approach.

For any $R > 0$, we denote by B_R the open ball of \mathbb{R}^d of radius R centered at the origin, and $B := B_1$. Let $\Gamma_R := \partial B_R$ and $n_R(x)$ be the normal unitary vector of Γ_R at the point $x \in \Gamma_R$ pointing outwards B_R . We introduce the vector spaces

$$V := \left\{ v \in L^2_{\text{loc}}(\mathbb{R}^d), \nabla v \in \left(L^2(\mathbb{R}^d) \right)^d \right\} \quad \text{and} \quad V_0 := \left\{ v \in V, \int_B v = 0 \right\}.$$

The space V_0 , endowed with the scalar product $\langle \cdot, \cdot \rangle$ defined by $\forall v, w \in V_0, \langle v, w \rangle := \int_{\mathbb{R}^d} \nabla v \cdot \nabla w$, is a Hilbert space.

For any matrix-valued field $\mathbb{A} \in L^\infty(\mathbb{R}^d, \mathcal{M}_{\alpha,\beta})$, any $R > 0$, any constant matrix $A \in \mathcal{M}_{\alpha,\beta}$, and any vector $p \in \mathbb{R}^d$, we denote by $w_p^{R,\mathbb{A},A}$ the unique solution in V_0 to

$$\boxed{-\text{div}\left(\mathbb{A}_{R,A}(p + \nabla w_p^{R,\mathbb{A},A})\right) = 0 \text{ in } \mathcal{D}'(\mathbb{R}^d),} \tag{7}$$

where (see Fig. 1)

$$\mathbb{A}_{R,A}(x) := \begin{cases} \mathbb{A}(x) & \text{if } x \in B_R, \\ A & \text{if } x \in \mathbb{R}^d \setminus B_R. \end{cases}$$

In (7), we keep the original coefficient \mathbb{A} in the ball B_R , and replace it outside B_R by a uniform coefficient A .

Assume that the matrix-valued field $\mathbb{A} \in L^\infty(\mathbb{R}^d, \mathcal{M}_{\alpha,\beta})$ satisfies the following:

Assumption 2.1. The rescaled matrix-valued fields \mathbb{A}^R , defined by $\mathbb{A}^R(x) = \mathbb{A}(Rx)$, form a family $(\mathbb{A}^R)_{R>0}$ that G -converges to a constant matrix $A^* \in \mathcal{M}_{\alpha,\beta}$ on B as R tends to infinity.

Under this assumption, the motivation for considering problems of the form (7) is twofold. First, we show in Section 3 below that the solution $w_p^{R,\mathbb{A},A}$ to (7) can be used to define consistent approximations of A^* . Second, in some cases, problem (7) can be efficiently solved, using a numerical approach directly inspired from that proposed in [6,15]. This is for example the case when, in B_R ,

$$\mathbb{A}(x) = \begin{cases} A_{\text{int}}^i I_d & \text{if } x \in B_R \cap B(x_i, r_i), \quad 1 \leq i \leq I, \quad I \in \mathbb{N}^*, \\ A_{\text{ext}} I_d & \text{if } x \in B_R \setminus \bigcup_{i=1}^I B(x_i, r_i), \end{cases} \tag{8}$$

where I_d is the identity matrix of $\mathbb{R}^{d \times d}$, $A_{\text{int}}^i, A_{\text{ext}} \in [\alpha, \beta]$ for any $1 \leq i \leq I$, $(x_i)_{1 \leq i \leq I} \subset B_R$ and $(r_i)_{1 \leq i \leq I}$ is some set of positive real numbers such that $\bigcup_{i=1}^I B(x_i, r_i) \subset B_R$ and $B(x_i, r_i) \cap B(x_j, r_j) = \emptyset$ for all $1 \leq i \neq j \leq I$. We have denoted by $B(x_i, r_i) \subset \mathbb{R}^d$ the ball of radius r_i centered at x_i . We refer to [5] for other cases.

The expression (8) corresponds to the case of (possibly stochastic) heterogeneous materials composed of spherical inclusions. The properties of the inclusions (i.e. the coefficients A_{int}^i), their centers x_i and their radii r_i may be random, as long as \mathbb{A} is stationary (see Fig. 1).

In the case (8), problem (7) can be efficiently solved using a boundary integral method (see [5]). Since $\mathbb{A}_{R,A}$ is uniform in each $B(x_i, r_i)$, in $B_R \setminus \bigcup_i B(x_i, r_i)$ and in $\mathbb{R}^d \setminus B_R$, problem (7) can indeed be recast as an integral equation on the spheres $\partial B(x_i, r_i)$ and Γ_R . In the case of random homogenization, the practical consequence is that, for the same number of degrees of freedom, we can afford to work on domains B_R that are much larger than the truncated domains Q_N in (5)–(6). We thus expect to obtain better approximations of A^* .

3. New definitions of approximate homogenized matrices

Assume that the matrix field \mathbb{A} satisfies [Assumption 2.1](#). We wish to use solutions to (7) to construct a family $(A^{*,R})_{R>0}$ that converges to the homogenized matrix A^* as R tends to infinity.

In the subsequent Sections 3.1, 3.2 and 3.3, we respectively present three possible choices leading to converging approximations, namely (12), (13), and (15). We refer to [5] for the proof of the results stated below. To introduce these choices, we note that the solution $w_p^{R,\mathbb{A},A}$ to (7) is equivalently the unique solution to the optimization problem

$$w_p^{R,\mathbb{A},A} = \operatorname{argmin}_{v \in V_0} J_p^{R,\mathbb{A},A}(v),$$

where

$$J_p^{R,\mathbb{A},A}(v) := \frac{1}{2|B_R|} \int_{B_R} (p + \nabla v)^T \mathbb{A} (p + \nabla v) + \frac{1}{2|B_R|} \int_{\mathbb{R}^d \setminus B_R} (\nabla v)^T A \nabla v - \frac{1}{|B_R|} \int_{\Gamma_R} (Ap \cdot n_R) v. \tag{9}$$

We set $\mathcal{J}_p^{R,\mathbb{A}}(A) := J_p^{R,\mathbb{A},A}(w_p^{R,\mathbb{A},A}) = \min_{v \in V_0} J_p^{R,\mathbb{A},A}(v)$. The linearity of the mapping $\mathbb{R}^d \ni p \mapsto w_p^{R,\mathbb{A},A} \in V_0$ yields that, for any $A \in \mathcal{M}_{\alpha,\beta}$, there exists a unique symmetric matrix $G^{R,\mathbb{A}}(A) \in \mathbb{R}^{d \times d}$ such that

$$\forall p \in \mathbb{R}^d, \quad \frac{1}{2} p^T G^{R,\mathbb{A}}(A) p = \mathcal{J}_p^{R,\mathbb{A}}(A).$$

(10)

Note that $\frac{1}{2} \operatorname{Tr} \left(G^{R,\mathbb{A}}(A) \right) = \sum_{i=1}^d \mathcal{J}_{e_i}^{R,\mathbb{A}}(A)$, where $(e_i)_{1 \leq i \leq d}$ is the canonical basis of \mathbb{R}^d . The following expression of $\mathcal{J}_p^{R,\mathbb{A}}(A)$ is useful:

$$\mathcal{J}_p^{R,\mathbb{A}}(A) = \frac{1}{2|B_R|} \int_{B_R} p^T \mathbb{A} p - \frac{1}{2|B_R|} \int_{B_R} (\nabla w_p^{R,\mathbb{A},A})^T \mathbb{A} \nabla w_p^{R,\mathbb{A},A} - \frac{1}{2|B_R|} \int_{\mathbb{R}^d \setminus B_R} (\nabla w_p^{R,\mathbb{A},A})^T A \nabla w_p^{R,\mathbb{A},A}. \tag{11}$$

Before describing our three approaches, we recall the following classical definition (see [16]):

Definition 3.1 (*G-convergence*). Let D be an open bounded smooth subdomain of \mathbb{R}^d . A family of matrix-valued functions $(\mathbb{A}^R)_{R>0} \subset L^\infty(D, \mathcal{M}_{\alpha,\beta})$ is said to *G-converge* in D to a matrix-valued function $\mathbb{A}^* \in L^\infty(D, \mathcal{M}_{\alpha,\beta})$ if, for all $f \in H^{-1}(D)$, the family $(u^R)_{R>0}$ of solutions to

$$-\operatorname{div} \left(\mathbb{A}^R \nabla u^R \right) = f \text{ in } \mathcal{D}'(D), \quad u^R \in H_0^1(D),$$

satisfies

$$u^R \rightharpoonup u^* \text{ weakly in } H_0^1(D), \quad \mathbb{A}^R \nabla u^R \rightharpoonup \mathbb{A}^* \nabla u^* \text{ weakly in } L^2(D),$$

where u^* is the unique solution to the homogenized equation

$$-\operatorname{div} \left(\mathbb{A}^* \nabla u^* \right) = f \text{ in } \mathcal{D}'(D), \quad u^* \in H_0^1(D).$$

3.1. First alternative definition: minimizing the scattering energy

To gain some intuition, we first recast (7) as

$$-\operatorname{div} \left[\left(A + \chi_{B_R} (\mathbb{A} - A) \right) \left(p + \nabla w_p^{R,\mathbb{A},A} \right) \right] = 0 \quad \text{in } \mathcal{D}'(\mathbb{R}^d),$$

where χ_{B_R} is the characteristic function of B_R . Thus, in this problem, the quantity $\mathbb{A} - A$ can be seen as a local perturbation to the homogeneous exterior medium characterized by the diffusion coefficient A . In turn, $w_p^{R,\mathbb{A},A}$ can be seen as the perturbation of an incident plane wave with wavevector p induced by the defect located in B_R . This is somehow reminiscent of the classical Eshelby problem [10]. A first idea is to choose a constant exterior matrix such that the scattering energy of the perturbation of the wave is as small as possible. We have the following result (recall that $G^{R,\mathbb{A}}$ is defined by (10)):

Lemma 3.2. For all $R > 0$ and $\mathbb{A} \in L^\infty(\mathbb{R}^d, \mathcal{M}_{\alpha,\beta})$, the function $\mathcal{M}_{\alpha,\beta} \ni A \mapsto \operatorname{Tr} \left(G^{R,\mathbb{A}}(A) \right)$ is concave.

It follows that, for any $R > 0$, there exists (at least) one matrix $A_1^R \in \mathcal{M}_{\alpha,\beta}$ such that

$$A_1^R = \operatorname{argmax}_{A \in \mathcal{M}_{\alpha,\beta}} \operatorname{Tr} \left(G^{R,\mathbb{A}}(A) \right). \tag{12}$$

This matrix A_1^R can be seen as a matrix which minimizes the scattering energy induced by the defect $\mathbb{A} - A$ of incident plane waves in an infinite medium. Indeed, using (11), we have that

$$A_1^R = \operatorname{argmin}_{A \in \mathcal{M}_{\alpha,\beta}} \sum_{i=1}^d \left(\int_{B_R} (\nabla w_{e_i}^{R,\mathbb{A},A})^T \mathbb{A} \nabla w_{e_i}^{R,\mathbb{A},A} + \int_{\mathbb{R}^d \setminus B_R} (\nabla w_{e_i}^{R,\mathbb{A},A})^T A \nabla w_{e_i}^{R,\mathbb{A},A} \right),$$

and the matrix A_1^R can thus be seen as a diffusion matrix A of the exterior medium such that the sum of the energies of the scattering waves with incident wavevectors e_i induced by the defect is minimal.

As shown in Proposition 3.3 below, the approximation A_1^R converges to A^* when $R \rightarrow \infty$.

3.2. Second alternative definition: an equivalent internal homogeneous material

We now introduce a second alternative definition of an approximate homogenized matrix:

$$A_2^R = G^{R,\mathbb{A}}(A_1^R), \tag{13}$$

where A_1^R is defined by (12). In view of (10), the above relation can also be written as $\forall p \in \mathbb{R}^d, \frac{1}{2} p^T A_2^R p = \mathcal{J}_p^{R,\mathbb{A}}(A_1^R)$. Using (9), the above definition can formally be recast as

$$\begin{aligned} & \int_{B_R} \left(p + \nabla w_p^{R,\mathbb{A},A_1^R} \right)^T \mathbb{A} \left(p + \nabla w_p^{R,\mathbb{A},A_1^R} \right) + \int_{\mathbb{R}^d \setminus B_R} \left(p + \nabla w_p^{R,\mathbb{A},A_1^R} \right)^T A_1^R \left(p + \nabla w_p^{R,\mathbb{A},A_1^R} \right) \\ &= \int_{B_R} p^T A_2^R p + \int_{\mathbb{R}^d \setminus B_R} p^T A_1^R p. \end{aligned} \tag{14}$$

The above relation is formal in the sense that both sides of the equation are infinite, but it nevertheless has an interesting physical interpretation. The above left-hand side corresponds to the energy of the heterogeneous material, modeled by \mathbb{A} in B_R and A_1^R outside of B_R , and where the field $p + \nabla w_p^{R,\mathbb{A},A_1^R}$ is solution to the equilibrium equation (7). Since $\nabla w_p^{R,\mathbb{A},A_1^R}$ is in $L^2(\mathbb{R}^d)$, its average is thought to vanish, and hence the average field is p . The above right-hand side corresponds to the energy of a material, modeled by A_2^R in B_R and A_1^R outside of B_R , in which the field is uniform and equal to p . The formal equation (14) thus “defines” A_2^R by an equality in terms of energies.

The following convergence result can be established:

Proposition 3.3. Assume that the matrix field \mathbb{A} satisfies Assumption 2.1. Then, the two families of matrices $(A_1^R)_{R>0}$ and $(A_2^R)_{R>0}$ respectively defined by (12) and (13), satisfy

$$A_1^R \xrightarrow{R \rightarrow +\infty} A^* \quad \text{and} \quad A_2^R \xrightarrow{R \rightarrow +\infty} A^*.$$

3.3. Third alternative definition: a self-consistent equation

We eventually introduce a third alternative definition, inspired by the approximation of A^* introduced in [7]. Assume that, for any $R > 0$, there exists a matrix $A_3^R \in \mathcal{M}_{\alpha,\beta}$ such that

$$A_3^R = G^{R,\mathbb{A}}(A_3^R). \tag{15}$$

Such a matrix formally satisfies the self-consistent equation

$$\begin{aligned} & \sum_{i=1}^d \int_{B_R} \left[\left(e_i + \nabla w_{e_i}^{R,\mathbb{A},A_3^R} \right)^T \mathbb{A} \left(e_i + \nabla w_{e_i}^{R,\mathbb{A},A_3^R} \right) - e_i^T A_3^R e_i \right] \\ &+ \int_{\mathbb{R}^d \setminus B_R} \left[\left(e_i + \nabla w_{e_i}^{R,\mathbb{A},A_3^R} \right)^T A_3^R \left(e_i + \nabla w_{e_i}^{R,\mathbb{A},A_3^R} \right) - e_i^T A_3^R e_i \right] = 0. \end{aligned}$$

This third definition also yields a converging approximation of A^* :

Proposition 3.4. Assume that the matrix field \mathbb{A} satisfies Assumption 2.1, and that there exists a sequence $(A_3^{R_k})_{k \in \mathbb{N}} \in (\mathcal{M}_{\alpha, \beta})^{\mathbb{N}}$ satisfying

$$\forall k \in \mathbb{N}, \quad A_3^{R_k} = G^{R_k, \mathbb{A}}(A_3^{R_k})$$

for some increasing sequence $(R_k)_{k \in \mathbb{N}}$ of positive numbers converging to $+\infty$. Then,

$$A_3^{R_k} \xrightarrow[k \rightarrow +\infty]{} A^*.$$

Note that we do not assume in this Proposition that the fixed-point equation (15) has a solution for all radii R . Proving the existence of a matrix A_3^R satisfying (15) in the general case is a delicate question. We however already have the following partial result, which addresses the isotropic case.

Proposition 3.5. Let $d \geq 2$. Let $\mathbb{A} \in L^\infty(\mathbb{R}^d, \mathcal{M}_{\alpha, \beta})$ be a matrix-valued field satisfying Assumption 2.1. Assume also that the homogenized matrix satisfies $A^* = a^* I_d$, where I_d is the identity matrix of $\mathbb{R}^{d \times d}$.

Then $a^* \in [\alpha, \beta]$ and, for any $R > 0$, there exists $a_3^R \in [\alpha, \beta]$ such that

$$a_3^R = \frac{1}{d} \text{Tr} \left(G^{R, \mathbb{A}}(a_3^R I_d) \right). \quad (16)$$

In addition,

$$a_3^R \xrightarrow[R \rightarrow +\infty]{} a^*.$$

Note that (16) is weaker than (15), which would read in this case $a_3^R I_d = G^{R, \mathbb{A}}(a_3^R I_d)$. However, this weaker condition is sufficient to prove that a_3^R is a converging approximation of a^* .

We conclude with the following two remarks. First, in the one-dimensional case, it is possible to obtain explicit expressions for A_1^R , A_2^R and A_3^R (which are uniquely defined by (12), (13) and (15), respectively) and see that they converge to A^* when $R \rightarrow \infty$. Second, in the case when \mathbb{A} is actually equal to a constant matrix A in B_R , then we have $A_1^R = A_2^R = A$, and the unique solution to (15) is $A_3^R = A$.

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