Arch. Mech., 49, 2, pp. 293–319, Warszawa 1997

Nonlinear transport equation and macroscopic properties of microheterogeneous media

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THE AIM of this paper is a study of the quasi-linear transport equation, for instance the stationary heat equation. For periodically microheterogeneous media, asymptotic homogenization has been performed with the local problem formulated as a minimization problem. The Hashin-Shtrikman type bounds and Golden–Papanicolaou integral representation theorem have been extended. In the case of layered composites, exact analytical formula for the effective coefficients have been derived. The possibility of applying Padé approximants and the Ritz method has been shown. Specific cases and examples have also been examined.

1. Introduction

THE NONLINEAR Eq. (2.1) below is here called a nonlinear transport equation. It is obvious that from the physical point of view, the study of such an equation is very important. Typical examples are the stationary heat conduction and a nonlinear dielectric. The small parameter $\varepsilon > 0$ characterizes a microstructure of the material. We have thus to deal with composite materials. Performing homogenization or passing with ε to zero one obtains the homogenized (effective) coefficients a^e_{ij} $(i, j = 1, 2, 3)$. Of our main interest will be the periodic homogenization, cf. [1, 2]. We shall also extend to the nonlinear problem studied, the results due to GOLDEN and PAPANICOLAOU [20] on the integral representation of the effective coefficients in the linear case when $a_{ij}(y, \omega)(y \in \mathbb{R}^3, \omega \in \Omega)$ are stationary matrix-valued random fields; here $(\Omega, \mathcal{F}, \mathcal{P})$ is a probability space. Such an extension is possible since in the local problem the macroscopic field $u^{(0)}$, say the macroscopic temperature $T = u^{(0)}$ in the case of the heat conduction, plays the role of a parameter only. It is thus also possible to exploit the Hashin - Shtrikman variational principles and bounds, elaborated for the linear transport equation.

Extensive literature is concerned with the linear conductivity i.e. when the coefficients a^ε_{ij} do not depend on the solution u^ε. The reader may refer to [1–21] for more details on the results achieved so far. In contrast to the linear case, there seems to exist only a few papers on the homogenization of the quasi-linear Eq. (2.1), cf. [22–25]. Those papers are purely theoretical and provide no examples of applications to composite materials. Also, the problem of the estimation of the effective coefficients has been left open, though a particular case has been studied by MITYUSHEV [26]. However, the definition of the effective conductivity used by this author is different from the formula obtained by homogenization. We observe that a^e_{ij} depend on $u^{(0)}$, where $u^{(0)}$ is a weak limit of u^ε when $\varepsilon \to 0$.

For instance, in the case of the heat conduction, a^{ε}_{ij} depend on the macroscopic temperature T. Such a dependence is in general a nonlinear one, even then when in each of phases constituting the composite a^{ε}_{ij} depend linearly on T; specific examples are provided in Secs. 5, 6 and 7 of our paper. A nonlinear dependence of the conductivities on the temperature is of vital importance not only in the study of engineering materials and structures [27, 28], but also for modelling the behaviour of biological tissues [29, 30].

The determination of the effective coefficients a^{e}_{ij} is of interest not only for undeformable bodies; such a problem arises quite naturally as an independent problem in the study of thermo- and piezo-electric composites [31, 32] and in thermodiffusion [33].

The objective of this paper is to study the quasi-linear heat equation (2.1) and provide some applications. Brief description of the contents of the paper reveals very well our aim. In Sec. 2 the method of two-scale asymptotic expansions is used in order to derive in a rather simple manner the homogenized coefficients $a^{e}_{ij}(u^{(0)})$; in the case of heat conduction $u^{(0)} = T$. The formulation of the local problem in the form of a minimization problem, in which the macroscopic field $u^{(0)}$ (for instance T) plays the role of a parameter is also delivered. In Sec. 3 variational principles and bounds of the Hashin - Shtrikman type are given. Section 4 deals with a straightforward extension of the GOLDEN - PAPANICOLAOU [19] representation theorem to the investigated quasi-linear problem. This theorem provides an integral representation of the effective coefficients $a^{e}_{ij}(u^{(0)})$ for two-component composites made of isotropic materials. In Sec. 5 analytical formulae for the homogenized coefficients of layered composites are derived. Section 6 reveals a possibility of an application of the Ritz method to the determination of local functions. A specific two-dimensional problem is also given. In the last section it is shown how to apply the powerful tool of Padé approximants to finding bounds on the effective coefficients.

2. Homogenization of quasi-linear heat equation with periodic coefficients

Let $V \subset \mathbb{R}^3$ be a bounded regular domain and $\Gamma = \partial V$ its boundary. We introduce a parameter $\varepsilon = l/L$, where l, L are typical length scales associated with microinhomogeneities and the region V, respectively.

We shall study the quasi-linear transport equation

$$\tag{2.1} \begin{aligned} -\frac{\partial}{\partial x_i}\left(a^{\varepsilon}_{ij}(x, u^{\varepsilon})\frac{\partial u^{\varepsilon}}{\partial x_j}\right) &= f \qquad \text{in} \quad V, \\ u^{\varepsilon}|_{\Gamma} &= 0 \qquad \text{on} \quad \Gamma, \end{aligned}$$

where $a^{\varepsilon}_{ij}(x, u^{\varepsilon}) = a_{ij}\left(\dfrac{x}{\varepsilon}, u^{\varepsilon}\right)$, $x \in V$. By Y we denote the so-called basic cell [1, 2], for instance $Y = (0, Y_1)\times(0, Y_2)\times(0, Y_3)$. For the sake of simplicity we assume that $a_{ij} = a_{ji}$, $i, j = 1, 2, 3$. As usual, we apply the summation convention. The material coefficients $a_{ij}(y, r)$ are Y-periodic in the first argument. More precisely,

$$a_{ij} : (y, r) \to a_{ij}(y, r),$$
$$\mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}$$

are assumed to satisfy the following conditions:

(i) For each $r \in \mathbb{R}$, $y \to a_{ij}(y, r)$ are mesurable and Y-periodic functions.

(ii) There exists a constant $\alpha > 0$ such that for every $r \in \mathbb{R}$, i.e. $y \in Y$ and for all $i, j = 1, 2, 3$, $|a_{ij}(y, r)| \leq \alpha$.

(iii) There exists a constant $k > 0$ such that

$$|a_{ij}(y, r_1) - a_{ij}(y, r_2)| \leq k|r_1 - r_2|,$$

for all $y \in \mathbb{R}^3$ and $r_1, r_2 \in \mathbb{R}$.

(iv) There exists $\alpha_0 > 0$ such that

$$a_{ij}(y, r)\xi_i\xi_j \geq \alpha_0|\xi|^2,$$

for all $\xi \in \mathbb{R}^3$ and $r \in \mathbb{R}$.

We note that for a fixed $\varepsilon > 0$ the material functions $a^{\varepsilon}_{ij}(x, r) = a_{ij}\left(\dfrac{x}{\varepsilon}, r\right)$ are εY-periodic in $x \in V$. After passage to the limit as $\varepsilon \to 0$, the homogenized coefficients a^{e}_{ij} will be obtained.

2.1. Method of two-scale asymptotic expansions

According to this method we make the following assumption (*ansatz*), cf. [1, 2]

$$u^{\varepsilon}(x) = u^{(0)}(x, y) + \varepsilon\, u^{(1)}(x, y) + \varepsilon^2\, u^{(2)}(x, y) + \cdots\,, \tag{2.2}$$

where $y = x/\varepsilon$, and the functions $u^{(0)}(x, \cdot)$, $u^{(1)}(x, \cdot)$, $u^{(2)}(x, \cdot)$, etc. are Y-periodic. Then we may write

$$\begin{aligned} a_{ij}(y, u^{(0)} + \varepsilon u^{(1)} + \varepsilon^2 u^{(2)} + \cdots) &= a_{ij}(y, u^{(0)}) + \varepsilon u^{(1)} \frac{\partial a_{ij}(y, u^{(0)})}{\partial u^{(0)}} \\ &+ \varepsilon^2 \left(u^{(2)}(x, y) \frac{\partial a_{ij}(y, u^{(0)})}{\partial u^{(0)}} + \frac{1}{2}(u^{(1)}(x, y))^2 \frac{\partial^2 a_{ij}(y, u^{(0)})}{\partial^2 u^{(0)}} \right) + \cdots\,. \end{aligned}$$

It is tacitly assumed that all derivatives appearing in the procedure of asymptotic homogenization make sense. We recall that for a function $f(x, y)$, where $y = x/\varepsilon$, the differentiation operator $\partial/\partial x_i$ should be replaced by $\dfrac{\partial}{\partial x_i} + \dfrac{1}{\varepsilon}\dfrac{\partial}{\partial y_i}$. According to the method of asymptotic expansions we compare the terms associated with the same power of ε. Proceeding similarly as in the linear case we successively obtain:

$\underline{\varepsilon^{-2}}$

$$\frac{\partial}{\partial y_j}\left(a_{ij}(y, u^{(0)}(x,y))\frac{\partial u^{(0)}(x,y)}{\partial y_i}\right) = 0.$$

This equation will be satisfied provided that $u^{(0)}$ does not depend on the local variable y, i.e. $u^{(0)} = u^{(0)}(x)$. This statement holds true under the assumption that the coefficients $a_{ij}(\cdot, u^{(0)}(x,\cdot))$ are Y-periodic.

$\underline{\varepsilon^{-1}}$

$$\frac{\partial}{\partial y_j}\left(a_{ij}(y, u^{(0)}(x))\left(\frac{\partial u^{(1)}(x,y)}{\partial y_i} + \frac{\partial u^{(0)}(x)}{\partial x_i}\right)\right) = 0.$$

$\underline{\varepsilon^{0}}$ (after integration over Y)

$$\frac{\partial}{\partial x_j}\left(\frac{1}{|Y|}\int\limits_Y a_{ij}(y, u^{(0)}(x))\left(\frac{\partial u^{(1)}(x,y)}{\partial y_i} + \frac{\partial u^{(0)}(x)}{\partial x_i}\right)dY\right) = -f(x),$$

where

$$u^{(1)}(x,y) = \frac{\partial u^{(0)}(x)}{\partial x_k}\chi^{(k)}(y, u^{(0)}).$$

The local functions $\chi^{(k)}(y, u^{(0)})$ are solutions to the local problem

$$\frac{\partial}{\partial y_j}\left(a_{ij}(y, u^{(0)})\left(\frac{\partial \chi^{(k)}(y, u^{(0)})}{\partial y_i} + \delta_{ik}\right)\right) = 0. \tag{2.3}$$

Let us introduce the space of Y-periodic functions defined by

$$H_{\text{per}}(Y) = \Big\{\phi \in H^1(Y) | \phi \text{ assumes equal values at the opposite faces of } Y\Big\}. \tag{2.4}$$

The weak (variational) formulation of Eq. (2.3) reads: find $\chi^{(k)}(\cdot, u^{(0)}) \in H_{\text{per}}(Y)$ such that

$$\int\limits_Y \left[a_{ij}(y, u^{(0)})\left(\frac{\partial \chi^{(k)}(y, u^{(0)})}{\partial y_i} + \delta_{ik}\right)\right]\frac{\partial v(y)}{\partial y_j}dy = 0, \tag{2.5}$$

for each $v \in H_{\text{per}}(Y)$. Then the homogenized equation has the following form

$$-\frac{\partial}{\partial x_j}\left(a^{e}_{ij}(u^{(0)})\frac{\partial u^{(0)}}{\partial x_i}\right) = f, \tag{2.6}$$

where the homogenized (effective) coefficients are given by

$$a^e_{ij}(u^{(0)}) = \frac{1}{|Y|}\int_Y \left[a_{ij}(y, u^{(0)}) + a_{kj}(y, u^{(0)})\frac{\partial \chi^{(i)}}{\partial y_k}\right] dy. \tag{2.7}$$

In the case of the heat conduction $u^{(0)} = T$, where T is the macroscopic temperature.

Both in (2.5) and (2.6) the transport coefficients satisfy only the earlier specified conditions (i) – (iv). We observe that in the local problem (2.5) $u^{(0)}$ plays the role of a parameter. This simple, but crucial observation means that (2.5) is equivalent to a convex minimization problem:

$$(\mathcal{P}_{\text{loc}}) \left| \begin{array}{l} \text{Find} \\ W(u^{(0)}, \mathbf{E}) = \inf\left\{ \dfrac{1}{2|Y|}\displaystyle\int_Y a_{ij}(y, u^{(0)})\left(\frac{\partial v}{\partial y_i} + E_i\right)\left(\frac{\partial v}{\partial y_j} + E_j\right) dy \;\; \middle| \right. \\ \hfill \left. v \in H_{\text{per}}(Y) \right\} \end{array} \right.$$

provided that $a_{ij} = a_{ji}$; here $E_i = \partial u^{(0)}/\partial x_i$. A solution $\overline{v} \in H_{\text{per}}(Y)$ exists and is unique up to a constant $c(u^{(0)})$. Due to linearity of $\overline{v}$ with respect to $\mathbf{E} = (E_i)$ we may write

$$\overline{v}(y, u^{(0)}) = \chi^{(k)}(y, u^{(0)})E_k\,. \tag{2.8}$$

In contrast to the local problem ($\mathcal{P}_{\text{loc}}$), problem (2.1) *cannot* be formulated as a minimization problem. Note also that

$$W(u^{(0)}, \mathbf{E}) = \frac{1}{2}a^e_{ij}(u^{(0)})E_iE_j$$

is the macroscopic potential. For instance, for dielectric composites the macroscopic displacement vector $\mathbf{D} = (D_i)$ has the form

$$D_i = \frac{\partial W}{\partial E_i} = a^e_{ij}(u^{(0)})E_j\,, \tag{2.9}$$

where $u^{(0)}$ is the electric field, say φ and $E_i = -\partial\varphi/\partial x_i$ (the sign of E_i in ($\mathcal{P}_{\text{loc}}$) is not important in the sense that one may consider either $\chi^{(k)}$ or $(-\chi^{(k)})$).

Knowing that the local problem can be formulated as the minimization problem ($\mathcal{P}_{\text{loc}}$) we come to a *very important conclusion*: all the variational bound techniques, including Hashin – Shtrikman bounds, developed for the linear transport equation can be applied to the estimation of the effective coefficients (2.7). In the next section we shall provide more details.

2.2. Justification: G-convergence

From the mathematical point of view the results presented in the previous subsection are formal. Rigorous proof concerning the convergence when in Eq. (2.1) ε tends to zero have been given by ARTOLA, DUVAUT [22] and next extended in [23, 25] to the case of not necessarily periodic coefficients. Having in mind applications to physical problems we have assumed that $a_{ij} = a_{ji}$. In fact, to perform homogenization either by the asymptotic method or by the method of H-convergence, such a symmetry is not required, cf. [22, 23]. H-convergence is the G-convergence generalized to the case of nonsymmetric coefficients, cf. [1, 23–25] for more details. The main result of ARTOLA and DUVAUT [22] is summarized in the form of

THEOREM 1. *Under the assumptions* (i)–(iv) *and*

$$f \in L^2(V), \tag{2.10}$$

there exists a subsequence $u^{\varepsilon'}$ *of* u^{ε} *and* $p > 2$ *such that*

$$u^{\varepsilon'} \rightharpoonup u^{(o)} \quad \text{in } W_0^{1,p}(V) \quad \text{weakly}, \tag{2.11}$$

where $u^{(o)} \in W_0^{1,p}(V)$ *is a solution of* Eq. (2.6).

REMARK 1. A weak solution of Eq. (2.1) is sought in the space $H_0^1(V)$. The existence theorem provided by ARTOLA and DUVAUT [22] requires that $f \in W^{-1,p}(V)$; $p > 2$ depends on V, α, α_0 and space dimension. We observe that in [22] the coefficients a^{ε}_{ij} are not necessarily symmetric.

3. Hashin–Shtrikman variational principles and bounds

The local problem ($\mathcal{P}_{\rm loc}$) can be used for finding variational bounds on the effective coefficients $a^{e}_{ij}(u^{(0)})$ similarly as in the linear case. Consider the case of the heat conduction; then, according to our notations $u^{(0)} = T$. For the dielectric coefficients $a^{e}_{ij}(\varphi)$ the considerations which follow are quite similar.

In this and in the next section we are interested in composite materials made by mixing two isotropic materials with conductivities $\lambda_1(T)$ and $\lambda_2(T)$, $0 < \lambda_1(T) < \lambda_2(T)$, in specified proportions θ_1 and $\theta_2 = 1 - \theta_1$. The conductivity of the composite is then given by

$$\lambda(y,T) = \lambda_1(T)\psi_1(y) + \lambda_2(T)\psi_2(y), \tag{3.1}$$

where $\psi_1(y)$ and $\psi_2(y)$ denote the characteristic functions of the sets where λ equals λ_1 and λ_2, respectively. Then the volume fractions are

$$\theta_1 = \frac{1}{|Y|}\int\limits_Y \psi_1(y)\,dy, \qquad \theta_2 = \frac{1}{|Y|}\int\limits_Y \psi_2(y)\,dy. \tag{3.2}$$

The local problem takes the form

$$(3.3)\qquad <\mathbf{a}^e(T)\mathbf{E},\mathbf{E}> = \inf\left\{ \frac{1}{|Y|}\int\limits_Y \lambda(y,T)\left(\frac{\partial v}{\partial y_i}+E_i\right)\left(\frac{\partial v}{\partial y_i}+E_i\right)dy \;\Big|\; v\in H_{\mathrm{per}}(Y)\right\},$$

where $\mathbf{E}\in\mathbb{R}^3$ and $<\mathbf{a}^e(T)\mathbf{E},\mathbf{E}> = a^e_{ij}(T)E_iE_j$. Hence elementary bounds on $\mathbf{a}^e$ readily follow, cf. [3]

$$(3.4)\qquad \Lambda_1(T)\mathbf{I}\le \mathbf{a}^e(T)\le \Lambda_2(T)\mathbf{I},$$

where $\mathbf{I}=(\delta_{ij})$ and

$$(3.5)\qquad \Lambda_1(T) = \left[\frac{1}{|Y|}\int\limits_Y (\lambda(y,T))^{-1}\,dy\right]^{-1} = \left[(\lambda_1(T))^{-1}\theta_1 + (\lambda_2(T))^{-1}\theta_2\right]^{-1},$$

$$(3.6)\qquad \Lambda_2(T) = \frac{1}{|Y|}\int\limits_Y \lambda(y,T)\,dy = \lambda_1(T)\theta_1+\lambda_2(T)\theta_2\,.$$

Recall that if $\mathbf{A}$ and $\mathbf{B}$ are matrices, then $\mathbf{A}\ge\mathbf{B}$ means that $<\mathbf{AE},\mathbf{E}>\ge <\mathbf{BE},\mathbf{E}>$ for each $\mathbf{E}\in\mathbb{R}^3$.

We pass now to a brief discussion of Hashin – Shtrikman variational principles. We follow the paper by KOHN and MILTON [3], which is restricted to the linear case.

3.1. Variational principle for bounding $\mathbf{a}^e(T)$ from below and lower bound

Suppose that a "comparison medium" is characterized by a conductivity $\lambda^c(T)$, independent of $y\in Y$. If $\lambda^c(T)$ is restricted to the range $0<\lambda^c(T)<\lambda_1(T)$, then $\lambda(y,T)-\lambda^c(T)>0$ and proceeding similarly to KOHN and MILTON [3], we arrive at the variational principle of Hashin – Shtrikman type for bounding $\mathbf{a}^e(T)$ from below

$$(3.7)\qquad \frac{1}{2}<(\mathbf{a}^e(T)-\lambda^c(T)\mathbf{I})\,\mathbf{E},\mathbf{E}> = \sup_{\boldsymbol{\sigma}}\frac{1}{|Y|}\int\limits_Y\left[<\boldsymbol{\sigma},\mathbf{E}> - \frac{1}{2}(\lambda(y,T)-\lambda^c(T))^{-1}|\boldsymbol{\sigma}|^2 - \frac{1}{2\lambda^c(T)}<\boldsymbol{\sigma},\nabla_y\Delta_y^{-1}\mathrm{div}_y\boldsymbol{\sigma}>\right]dy.$$

Here $\boldsymbol{\sigma}=(\sigma_i)$ is a Y-periodic vector field and $|\boldsymbol{\sigma}|^2=\sigma_i\sigma_i$; moreover $(\nabla_y v)_i = \partial v/\partial y_i$ and Δ_y denotes the Laplacian with respect to y, while Δ_y^{-1} is its inverse.

To derive from (3.7) the Hashin - Shtrikman type lower bound, the test field $\boldsymbol{\sigma}$ is chosen in the form

$$\boldsymbol{\sigma}(y) = \psi_2(y)\boldsymbol{\eta}, \tag{3.8}$$

where $\boldsymbol{\eta}$ is a constant vector.

Following KOHN and MILTON [3] we finally obtain

$$\operatorname{tr}\left[(\mathbf{a}^e(T) - \lambda_1(T)\mathbf{I})^{-1}\right] \leq \frac{n}{(\lambda_2(T) - \lambda_1(T))\theta_2} + \frac{1-\theta_2}{\lambda_1(T)\theta_2} = \frac{n-1}{\Lambda_2(T) - \lambda_1(T)} + \frac{1}{\Lambda_1(T) - \lambda_1(T)}, \tag{3.9}$$

where $\operatorname{tr}\mathbf{A} = A_{ii}$ and n denotes the space dimension ($n = 3$ in the three-dimensional case).

3.2. Variational principle for bounding $\mathbf{a}^e(T)$ from above and upper bound

If $\lambda^c(T)$ is restricted to the range $\lambda_2(T) < \lambda^c(T) < \infty$, then $\lambda(y,T) - \lambda^c(T)$ is negative and the Hashin - Shtrikman type variational principle for bounding $\mathbf{a}^e(T)$ from above has the following form

$$\frac{1}{2} < (\mathbf{a}^e(T)\mathbf{E}, \mathbf{E} >= \inf_{\boldsymbol{\sigma}} \frac{1}{|Y|} \int_Y \left[< \boldsymbol{\sigma}, \mathbf{E} > -\frac{1}{2}(\lambda(y,T) - \lambda^c(T))^{-1} |\boldsymbol{\sigma}|^2 - \frac{1}{2\lambda^c(T)} < \boldsymbol{\sigma}, \nabla_y \Delta_y^{-1} \operatorname{div}_y \boldsymbol{\sigma} > \right] dy. \tag{3.10}$$

Substituting

$$\boldsymbol{\sigma}(y) = \psi_1(y)\boldsymbol{\eta} \tag{3.11}$$

into (3.10) and proceeding similarly as in [3] we obtain that

$$\operatorname{tr}\left[(\lambda_2(T)\mathbf{I} - \mathbf{a}^e(T))^{-1}\right] \leq \frac{n}{(\lambda_2(T) - \lambda_1(T))\theta_1} - \frac{1-\theta_1}{\lambda_2(T)\theta_2} = \frac{n-1}{\lambda_2(T) - \Lambda_2(T)} + \frac{1}{\lambda_2(T) - \Lambda_1(T)}. \tag{3.12}$$

4. Two-phase isotropic composites and integral representation of the homogenized coefficients

BOCCARDO and MURAT [23] have studied the convergence of solutions of Eq. (2.1) without the assumption of periodicity of the coefficients $a_{ij}^\varepsilon(\cdot, u^\varepsilon)$; the symmetry of those coefficients has also not been required. Under some conditions, it has been shown that

(4.1) $$\mathbf{a}^{\varepsilon}(\cdot, r) \xrightarrow{H} \overline{\mathbf{a}}(\cdot, r) \qquad (r - \text{fixed}, \quad \varepsilon \to 0).$$

Here H denotes "H-convergence". In the case of periodic coefficients, we obviously have $\overline{\mathbf{a}}(x, r) = \mathbf{a}^e(r)$, where $\mathbf{a}^e(r)$ is given by (2.7); $r \in \mathbb{R}$. To find $\overline{\mathbf{a}}(x, r)$ one needs additional information on the microstructure (we observe, that in the general case the effective coefficients may still depend on the macroscopic variable $x \in V$). For instance, such an information is available for statistically homogeneous ergodic (S.H.E) media [34]. Stochastically periodic media are a specific case of S.H.E. media. For more information on stochastic homogenization the reader should refer to [19] and to the references cited therein. Our aim in this section is not to discuss the stochastic homogenization of Eq. (2.1), which can be done by a straightforward extension of the results due to PAPANICOLAOU and VARADHAN [18] as well as to GOLDEN and PAPANICOLAOU [19]. Instead, we are going to continue the study of periodic homogenization of two-phase isotropic composites. As it has been observed by SAB [34], periodic media are a special case of S.H.E. media. Indeed, for periodic media the probability space $(\Omega, \mathcal{F}, \mathcal{P})$ is defined by the basic cell: $\Omega = [0, Y_1) \times [0, Y_2) \times [0, Y_3)$ if $Y = (0, Y_1) \times (0, Y_2) \times (0, Y_3)$; $\mathcal{F}$ is the Lebesgue σ-algebra and $P = \frac{1}{|Y|} dy$. It means that the results obtained in [18, 19] are also valid for the case of periodic homogenization. Particularly, recalling that in Eq. (2.7) the macroscopic field $u^{(0)}$ plays the role of a parameter, we can extend the integral representation formula due to GOLDEN and PAPANICOLAOU [19], cf. also [20, 21]. For a two-phase composite made of isotropic materials we write

(4.2) $$a_{ij}(y, u^{(0)}) = a(y, u^{(0)})\delta_{ij}\,,$$

where, for a fixed $u^{(0)}$, $a(y, u^{(0)})$ assumes only two values $a_1(u^{(0)})$ and $a_2(u^{(0)})$ with $0 < a_1(u^{(0)}) < a_2(u^{(0)})$. Thus we have, cf. (3.1)

(4.3) $$a(y, u^{(0)}) = a_1(u^{(0)})\psi_1(y) + a_2(u^{(0)})\psi_2(y).$$

Hence we conclude that important is only the ratio

(4.4) $$h(u^{(0)}) = \frac{a_2(u^{(0)})}{a_1(u^{(0)})} \qquad \left(\text{or} \quad h(u^{(0)}) = \frac{a_1(u^{(0)})}{a_2(u^{(0)})}\right).$$

In view of Eq. (2.7) we write

(4.5) $$a^e_{ij}(u^{(0)}) = a_1(u^{(0)}) \int_Y \left[\psi_1(y) + h(u^{(0)})\psi_2(y)\right] \widetilde{E}^{(i)}_j \, dy,$$

where $\widetilde{E}_j^{(i)} = \dfrac{\partial \chi^{(i)}(y, u^{(0)})}{\partial y_j} + \delta_{ij}$ provided that $Y = (0,1)^3$ (for the sake of simplicity). Thus the effective transport coefficients are functions of $h(u^{(0)})$; we write $a^e_{ij}(u^{(0)}) = \widetilde{a}_{ij}(h(u^{(0)}))$.

Suppose now that $h(u^{(0)})$ is a complex variable, cf. [19]. It means that the coefficients $a_1(u^{(0)})$ and $a_2(u^{(0)})$ are treated as complex-valued coefficients. Physically, imaginary parts characterize dissipative properties of the composite.

From the mathematical point of view, it is then possible to apply the theorem on the resolvent representation [19–21].

PROPOSITION 1. The function $\widetilde{a}_{ij}$ is an analytic function of the complex variable $h(u^{(0)})$ everywhere except on the negative real axis.

P r o o f. For $u^{(0)}$ fixed, it is similar to the one given in [19], provided that in the formula (4.7) of the last paper one takes $\mathcal{P}(d\omega) = dy$, $\Omega = Y$ (more precisely $\Omega = [0,1)^3$). $\square$

Equation (4.5) may be written as follows

$$m_{ij}(h(u^{(0)})) = \frac{a^e_{ij}(u^{(0)})}{a_1(u^{(0)})} = \int\limits_Y \left[\psi_1(y) + h(u^{(0)})\psi_2(y)\right] \widetilde{E}_j^{(i)}\, dy. \tag{4.6}$$

Now we are in a position to state the main result of this section

THEOREM 2 (REPRESENTATION FORMULA). *Let*

$$s(u^{(0)}) = \frac{1}{1 - h(u^{(0)})}, \qquad F_{ij}(s(u^{(0)})) = \delta_{ij} - m_{ij}(h(u^{(0)})). \tag{4.7}$$

There exist finite Borel measures $\mu_{ij}(dz)$ defined for $0 \le z \le 1$ such that the diagonals $\mu_{ii}(dz)$ (no summation over i) are positive measures satisfying

$$F_{ij}(s(u^{(0)})) = \int\limits_0^1 \frac{\mu_{ij}(dz)}{s(u^{(0)}) - z}, \qquad i, j = 1, 2, 3 \tag{4.8}$$

for all complex $s(u^{(0)})$ outside $0 \le \mathrm{Re}\, s(u^{(0)}) \le 1$, $\mathrm{Im}\, s(u^{(0)}) = 0$.

P r o o f. For a fixed $u^{(0)}$ it is quite similar to the proof of the representation formula given by GOLDEN and PAPANICOLAOU [19], where h, $\mathcal{P}(d\omega)$, s and L_i should by replaced by $h(u^{(0)})$, dy, $s(u^{(0)})$ and $\partial/\partial y_i$, respectively.

COROLLARY 1. Suppose that the medium is macroscopically isotropic. Then $m_{ij}\left(h(u^{(0)})\right) = m(h(u^{(0)}))\delta_{ij}$ and

$$1 - m(h(u^{(0)})) = F(s(u^{(0)})) = \int\limits_0^1 \frac{\mu(dz)}{s(u^{(0)}) - z}, \quad s(u^{(0)}) \text{ outside } [0,1]. \tag{4.9}$$

In the literature, one can find alternative forms of the integral in the r.h.s. of the last relation like the one we shall use in the next section, cf. also [35]

$$m(h(u^{(0)})) - 1 = \eta(u^{(0)})f_1(\eta(u^{(0)})), \tag{4.10}$$

where

$$f_1(\eta(u^{(0)})) = \int_0^1 \frac{\mu(dz)}{1+\eta(u^{(0)})z}, \qquad \eta(u^{(0)}) = h(u^{(0)}) - 1, \tag{4.11}$$

is a Stieltjes function defined in the cut $(-\infty \le \eta(u^{(0)}) \le -1)$ complex plane; here $s(u^{(0)}) = -(1/\eta(u^{(0)}))$.

Just this representation formula will be used in Sec. 7 for the determination of universal curves allowing for finding lower and upper bounds on the effective conductivity $\lambda_e(T)$ for an isotropic, heat conducting medium by applying Padé approximants.

REMARK 2. To the best of our knowledge, in the available literature a generalization of the very nice representation formula (4.8) to composites made of more than two isotropic components or of anisotropic materials is still lacking. Partial results have been presented in [20, 21] by using several complex variables.

5. Microperiodic layered composite

Layered composites are often used in engineering practice. In this section we shall derive the explicit form of the homogenized coefficients for the lamination in the direction y_1, provided that the composite is made of two materials. More general cases of layering can be treated similarly.

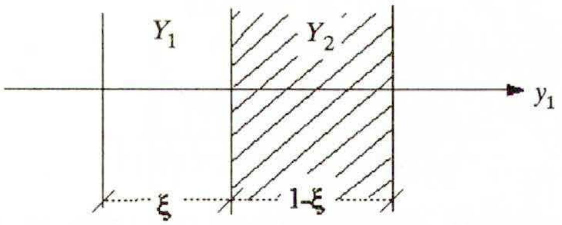

FIG. 1. Basic cell for two-phase layered composites.

Now the basic cell reduces to an interval, say (0,1). Thus the material coefficients of such a composite are specified by

$$a_{ij}(y,T) = \begin{cases} a_{ij}^{(1)}(T) & \text{if} \quad y_1 \in (0,\xi), \\ a_{ij}^{(2)}(T) & \text{if} \quad y_1 \in (\xi,1). \end{cases} \tag{5.1}$$

After lengthy, though simple calculations the local functions can be found in a closed form; they are piecewise linear, cf. [32, 33]

$$\frac{\partial \chi^{(k)}(y_1,T)}{\partial y_1} = \begin{cases} -(1-\xi)\frac{1}{A(\xi,T)}[\![a_{1k}(T)]\!] & \text{if} \quad y_1 \in (0,\xi), \\ \xi\frac{1}{A(\xi,T)}[\![a_{1k}(T)]\!] & \text{if} \quad y_1 \in (\xi,1). \end{cases} \tag{5.2}$$

From Eq. (2.7) we obtain the homogenized coefficients

$$a^{e}_{kl}(T) = < a_{kl}(y_1,T) > -\xi(1-\xi)\frac{1}{A(\xi,T)}[\![a_{1k}(T)]\!][\![a_{1l}(T)]\!], \tag{5.3}$$

where

$$\begin{aligned} < a_{kl}(y_1,T) > &= \xi a^{(1)}_{kl}(T) + (1-\xi)a^{(2)}_{kl}(T), \\ A(\xi,T) &= \xi a^{(2)}_{11}(T) + (1-\xi)a^{(1)}_{11}(T), \\ [\![a_{ij}(T)]\!] &= a^{(2)}_{ij}(T) - a^{(1)}_{ij}(T). \end{aligned}$$

If $a^{(1)}_{ij} = 0$ for $i \neq j$ and $a^{(2)}_{ij} = 0$ for $i \neq j$ then the coefficients $a^h_{11}(T)$, $a^h_{22}(T)$, $a^h_{33}(T)$ are given by

$$\begin{aligned} a^h_{11}(T) &= \frac{1}{\xi\dfrac{1}{a^{(1)}_{11}(T)} + (1-\xi)\dfrac{1}{a^{(2)}_{11}(T)}}, \\ a^h_{22}(T) &= < a_{22}(T,y) >, \qquad a^h_{33}(T) = < a_{33}(T,y) > . \end{aligned} \tag{5.4}$$

If we set

$$h(T) = \frac{a^{(1)}_{11}(T)}{a^{(2)}_{11}(T)},$$

then Eq. $(5.4)_1$ takes the form

$$\frac{a^h_{11}(T)}{a^{(2)}_{11}(T)} = \frac{h(T)}{\xi + (1-\xi)h(T)}. \tag{5.5}$$

Consider now a particular case by assuming that layers are made of isotropic materials while the dependence on the temperature is linear:

$$a_{ij}(y_1,T) = \begin{cases} \delta_{ij}(\alpha_1 + \beta_1 T) & \text{if} \quad y_1 \in (0,\xi), \\ \delta_{ij}(\alpha_2 + \beta_2 T) & \text{if} \quad y_1 \in (\xi,1). \end{cases} \tag{5.6}$$

Then we have

$$[\![a_{ij}]\!] = ([\![\alpha]\!] + [\![\beta]\!]T)\,\delta_{ij}, \tag{5.7}$$

and

$$a^e_{ij}(T) = \delta_{ij}\{[\xi\alpha_1 + (1-\xi)\alpha_2)] + T[\xi\beta_1 + (1-\xi)\beta_2]\} - \delta_{i1}\delta_{1j}\xi(1-\xi)\frac{[\alpha_2 - \alpha_1 + T(\beta_2 - \beta_1)]^2}{\xi\alpha_2 + (1-\xi)\alpha_1 + T[\xi\beta_2 + (1-\xi)\beta_1]}. \tag{5.8}$$

From the last relation we conclude that the only nontrivial homogenized coefficient is given by (the remaining effective coefficients are merely averages):

$$a^e_{11}(T) = a(\xi) + b(\xi)T + \frac{c(\xi)}{T - d(\xi)}, \tag{5.9}$$

where

$$\begin{aligned}
a(\xi) &= \overline{\alpha}(\xi) - \xi(1-\xi)\left[2\frac{[\![\alpha]\!][\![\beta]\!]}{\widetilde{\beta}(\xi)} - \widetilde{\alpha}(\xi)\left(\frac{[\![\beta]\!]}{\widetilde{\beta}(\xi)}\right)^2\right],\\
b(\xi) &= \overline{\beta}(\xi) - \xi(1-\xi)\frac{([\![\beta]\!])^2}{\widetilde{\beta}(\xi)},\\
c(\xi) &= -\frac{\xi(1-\xi)}{\widetilde{\beta}}\left([\![\alpha]\!] - [\![\beta]\!]\frac{\widetilde{\alpha}}{\widetilde{\beta}(\xi)}\right)^2,\\
d(\xi) &= \frac{\widetilde{\alpha}(\xi)}{\widetilde{\beta}(\xi)},
\end{aligned}$$

$$\overline{\alpha} = \xi\alpha_1 + (1-\xi)\alpha_2, \qquad \overline{\beta} = \xi\beta_1 + (1-\xi)\beta_2,$$

$$\widetilde{\alpha} = \xi\alpha_2 + (1-\xi)\alpha_1, \qquad \widetilde{\beta} = \xi\beta_2 + (1-\xi)\beta_1.$$

We note that though in both layers the conductivity coefficients depend linearly on the temperature, yet the dependence of a^e_{11} on T is nonlinear.

5.1. Temperature distribution in layered and homogenized composites

Let us investigate a two-phase isotropic composite consisting of n layers made of a material with the conductivity coefficient $\lambda_1(T) = \alpha_1 + \beta_1 T$ and n layers with the conductivity coefficient $\lambda_2(T) = \alpha_2 + \beta_2 T$, cf. Fig. 2.

The layers with odd and even numbers have the thickness l_1/n and l_2/n, respectively. Obviously, $l = l_1 + l_2$ denotes the thickness of the composite. The conductivity coefficient in the composite is thus given by

$$\lambda(x,T) = \begin{cases} \lambda_1(T) & \text{if } x \in \Delta_i \text{ and } i \text{ is odd,}\\ \lambda_2(T) & \text{if } x \in \Delta_i \text{ and } i \text{ is even,}\end{cases}$$

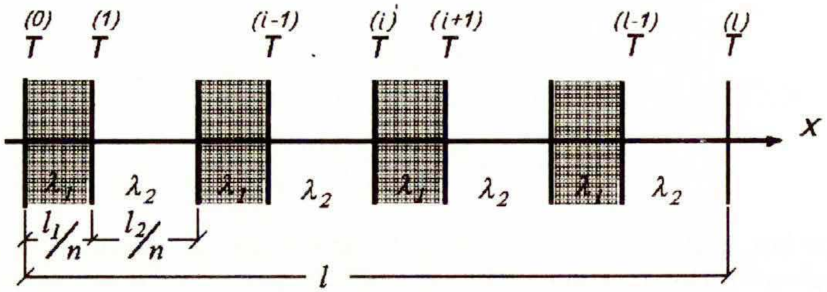

FIG. 2. Layered composite.

where $\Delta_i = (x_{i-1}, x_i)$; moreover

$$x_i = \begin{cases} \frac{l}{2n} i & \text{if } i \text{ is even}, \\ \frac{l}{2n}(i-1) + \frac{l_1}{n} & \text{if } i \text{ is odd}. \end{cases}$$

Denote by $\overset{(i)}{T}(x)$ the temperature distribution in the interval Δ_i; $\overset{(i-1)}{T}$ and $\overset{(i)}{T}$ are temperatures at the end point of Δ_i. The axis $0x$ is perpendicular to the layers.

The heat equation in the layers with odd numbers is given by

$$\frac{d}{dx}\left[\left(\alpha_1 + \beta_1 \overset{(i)}{T}(x)\right) \frac{d}{dx} \overset{(i)}{T}(x)\right] = 0. \tag{5.10}$$

Similarly, in the layers with even numbers we have

$$\frac{d}{dx}\left[\left(\alpha_2 + \beta_2 \overset{(i)}{T}(x)\right) \frac{d}{dx} \overset{(i)}{T}(x)\right] = 0. \tag{5.11}$$

Solving Eq. (5.10) we obtain

$$\overset{(i)}{T}(x) = \frac{1}{k_1}\left[1 - \sqrt{1 + 2k_1(\overset{(i)}{A}_1 x + \overset{(i)}{B}_1)}\right], \quad x \in \Delta_i \quad (i - \text{odd}), \tag{5.12}$$

where $k_1 = \beta_1/\alpha_1$ and

$$\overset{(i)}{A}_1 = \frac{n}{l_1}\left[\overset{(i)}{T} - \overset{(i-1)}{T} + \frac{k_1}{2}(\overset{(i)}{T}{}^2 - \overset{(i-1)}{T}{}^2)\right],$$

$$\overset{(i)}{B}_1 = \frac{n}{l_1}\left[x_i \overset{(i)}{T} - x_{i-1} \overset{(i-1)}{T} + \frac{k_1}{2}(x_i \overset{(i)}{T}{}^2 - x_{i-1} \overset{(i-1)}{T}{}^2)\right].$$

Similarly Eq. (5.11) yields

$$\overset{(i)}{T}(x) = \frac{1}{k_2}\left[1 - \sqrt{1 + 2k_2(\overset{(i)}{A_2}\,x + \overset{(i)}{B_2})}\right], \quad x \in \Delta_i \quad i - \text{even}, \tag{5.13}$$

where $k_2 = \beta_2/\alpha_2$ and

$$\overset{(i)}{A_2} = \frac{n}{l_2}\left[\overset{(i)}{T} - \overset{(i-1)}{T} + \frac{k_2}{2}(\overset{(i)}{T}{}^2 - \overset{(i-1)}{T}{}^2)\right],$$

$$\overset{(i)}{B_2} = \frac{n}{l_2}\left[x_i\,\overset{(i)}{T} - x_{i-1}\,\overset{(i-1)}{T} + \frac{k_2}{2}(x_i\overset{(i)}{T}{}^2 - x_{i-1}\,\overset{(i-1)}{T}{}^2)\right].$$

Assuming continuity of the heat flux at the points x_i $(i = 1, ..., 2n-1)$

$$\left(\alpha_1 + \beta_1\,\overset{(i)}{T}(x_i)\right)\frac{d}{dx}\,\overset{(i)}{T}(x_i) = \left(\alpha_2 + \beta_2\,\overset{(i+1)}{T}(x_i)\right)\frac{d}{dx}\,\overset{(i+1)}{T}(x_i), \quad i - \text{odd},$$

$$\left(\alpha_2 + \beta_2\,\overset{(i)}{T}(x_i)\right)\frac{d}{dx}\,\overset{(i)}{T}(x_i) = \left(\alpha_1 + \beta_1\,\overset{(i+1)}{T}(x_i)\right)\frac{d}{dx}\,\overset{(i+1)}{T}(x_i), \quad i - \text{even},$$

we obtain

$$\overset{(i)}{A_1} = \overset{(i+1)}{A_2} \quad \text{if } i \text{ is odd}, \qquad \overset{(i)}{A_2} = \overset{(i+1)}{A_1} \quad \text{if } i \text{ is even}.$$

Hence we derive the recurrence formula for the determination of $\overset{(i)}{T}$ $(i = 1, ..., 2n-1)$ provided that $\overset{(0)}{T}$ and $\overset{(l)}{T}$ are prescribed:

$$\overset{(i)}{T} = \begin{cases} -C + \sqrt{C^2 + \dfrac{2C}{l}\left[l_2\overset{(i+1)}{T} + l_1\overset{(i-1)}{T} + k_1 l_2 \overset{(i+1)}{T}{}^2 + k_2 l_1 \overset{(i-1)}{T}{}^2\right]}, & \text{for } i \text{ even}, \\[2ex] -C + \sqrt{C^2 + \dfrac{2C}{l}\left[l_2\overset{(i-1)}{T} + l_1\overset{(i+1)}{T} + k_1 l_2 \overset{(i-1)}{T}{}^2 + k_2 l_1 \overset{(i+1)}{T}{}^2\right]}, & \text{for } i \text{ odd}, \end{cases} \tag{5.14}$$

where

$$2C = \frac{l}{l_1 k_2 + l_2 k_1}.$$

In the interior of the intervals Δ_i the temperature is given by (5.12) and (5.13).

Now we shall compare the temperature at the interfaces with the (*one-dimensional*) homogenized solution. The homogenized equation has the form

$$\frac{d}{dx}\left[a_{11}^e(T(x))\frac{d}{dx}T(x)\right] = 0.$$

We recall that $a_{11}^{e}(T)$ is now specified by (5.9). Then the solution of the last (homogenized) equation is given by

$$aT + \frac{b}{2}T^2 + c\ln|T + d| = Ax + B, \tag{5.15}$$

where

$$A = \frac{1}{x_l - x_0}\left(a\left(\overset{(l)}{T} - \overset{(0)}{T}\right) + \frac{b}{2}\left(\overset{(l)}{T}{}^2 - \overset{(0)}{T}{}^2\right) + c\ln\left|\frac{\overset{(l)}{T} + d}{\overset{(0)}{T} + d}\right|\right),$$

$$B = \frac{1}{x_l - x_0}\left(a\left(x_l\overset{(0)}{T} - x_0\overset{(l)}{T}\right) + \frac{b}{2}\left(x_l\overset{(0)}{T}{}^2 - x_0\overset{(l)}{T}{}^2\right) + c\ln\left|\frac{\left(\overset{(l)}{T} + d\right)^{x_0}}{\left(\overset{(0)}{T} + d\right)^{x_l}}\right|\right)$$

provided that the boundary conditions are:

$$T(x_0) = \overset{(0)}{T}, \qquad T(x_l) = \overset{(l)}{T}.$$

5.2. Example

Let us assume that

$$\lambda_1(T) = 0.5 + 2T, \qquad \lambda_2(T) = 0.8 + 1.5T,$$

$$l = 10, \qquad n = 5, \qquad \frac{l_1}{l} = 0.4, \qquad \overset{(0)}{T} = 0, \qquad \overset{(l)}{T} = 15.$$

In Fig. 3 the dots denote the interface temperatures calculated according to (5.14). The continuous curve represents the temperature distribution obtained from the solution of the homogenized problem, cf. (5.15).

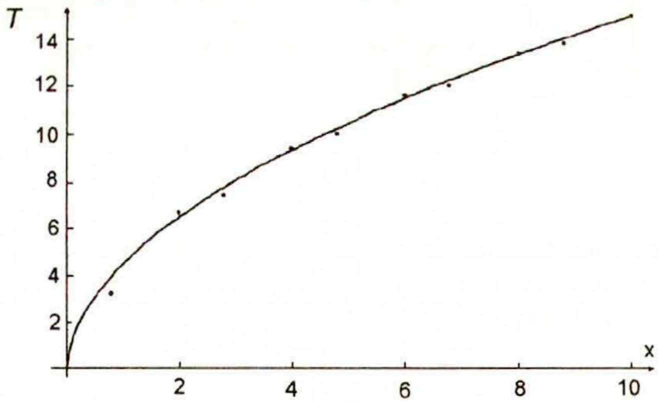

FIG. 3.

6. Ritz method

The Ritz method offers a possibility of determination of local functions in an approximate manner.

6.1. General case

We shall be looking for an approximate solution of the local problem by the Ritz method. Accordingly, we take, cf. [32, 33]

$$\chi^{(m)}(y,T) = \chi_a^{(m)}(T)\phi^a(y) = \sum_a \chi_a^{(m)}(T)\phi^a(y). \tag{6.1}$$

Here $\phi^a(y)$, $a = 1, 2, \ldots, \overline{a}$ are prescribed Y-periodic functions and $\chi_a^m(T)$ are unknown constants.

The local problem (2.5) should now be satisfied for test functions of the form

$$v = v_a \phi^a(y). \tag{6.2}$$

To determine the unknown constants one has to solve the following algebraic equations:

$$\chi_a^{(m)} A^{ab} = B^{mb}, \tag{6.3}$$

where

$$A^{ab}(T) = \int_Y a_{ij}(y,T)\phi^a_{,i}\phi^b_{,j}\, dy,$$

$$B^{ja}(T) = -\int_Y a_{ji}(y,T)\phi^a_{,i}\, dy,$$

with $\phi^a_{,i} = \dfrac{\partial \phi^a}{\partial y_i}$. For a given macroscopic temperature T the solution is

$$\chi_a^{(k)}(T) = (\mathbf{A}^{-1}(T))_{ab} B^{kb}(T).$$

Here $\mathbf{A}^{-1}$ is the inverse matrix of $\mathbf{A}$.

We finally obtain

$$a^e_{ij}(T) = < (a_{ij}(y,T) > + (\mathbf{A}^{-1}(T))_{ab} B^{ib}(T) B^{ja}(T). \tag{6.4}$$

6.2. Specific two-dimensional problem: two-phase composite

To illustrate the outlined general procedure we consider a two-phase composite material with the conductivity coefficients given by

$$a_{ij}(y,T) = \begin{cases} \lambda_1(T)\delta_{ij} & \text{if } y \in Y_1\,, \\ \lambda_2(T)\delta_{ij} & \text{if } y \in Y_2\,. \end{cases} \tag{6.5}$$

Now $y = (y_1, y_2)$, $\phi^a_{,3} = \dfrac{\partial \phi^a}{\partial y_3} = 0$ and $A^{a,b}(T)$ takes the form

$$A^{a,b}(T) = \lambda_2(T)F[a,b,i,i] - [\![\lambda(T)]\!]f[a,b,i,i], \tag{6.6}$$

$$B^{ja}(T) = [\![\lambda(T)]\!]f[a,j]. \tag{6.7}$$

Here

$$f[a,b,i,j] = \int\limits_{Y_1} \frac{\partial\phi^a}{\partial y_i}\frac{\partial\phi^b}{\partial_j} dy_1\,dy_2, \qquad F[a,b,i,j] = \int\limits_{Y} \frac{\partial\phi^a}{\partial y_i}\frac{\partial\phi^b}{\partial y_j} dy_1 dy_2, \tag{6.8}$$

$$f[a,i] = \int\limits_{Y_1} \frac{\partial\phi^a}{\partial y_i} dy_1\,dy_2, \qquad [\![\lambda(T)]\!] = \lambda_2(T) - \lambda_1(T).$$

Consider now a particular case of a square inclusion as presented in Fig. 4.

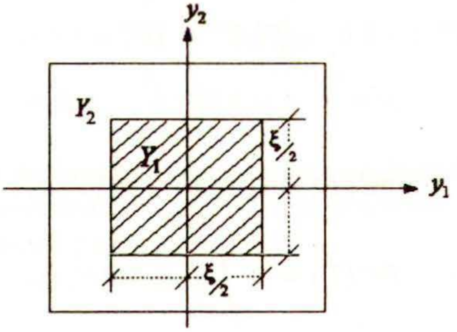

FIG. 4.

The base functions are assumed in the following form

$$\phi^1(y_1,y_2) = \begin{cases} \xi y_1 + \dfrac{\xi}{2} & \text{if } y_1 \in \left(-\dfrac{1}{2}, -\dfrac{\xi}{2}\right), \\ -(1-\xi)y_1 & \text{if } y_1 \in \left(-\dfrac{\xi}{2}, \dfrac{\xi}{2}\right), \\ \xi y_1 - \dfrac{\xi}{2} & \text{if } y_1 \in \left(\dfrac{\xi}{2}, \dfrac{1}{2}\right); \end{cases} \tag{6.9}$$

$$\phi^2(y_1,y_2) = \begin{cases} \xi y_2 + \dfrac{\xi}{2} & \text{if} \quad y_2 \in \left(-\dfrac{1}{2}, -\dfrac{\xi}{2}\right), \\ -(1-\xi)y_2 & \text{if} \quad y_2 \in \left(-\dfrac{\xi}{2}, \dfrac{\xi}{2}\right), \\ \xi y_2 - \dfrac{\xi}{2} & \text{if} \quad y_2 \in \left(\dfrac{\xi}{2}, \dfrac{1}{2}\right); \end{cases} \tag{6.10}$$

$$\phi^3(y_1,y_2) = \cos(\pi y_1)\sin(2\pi y_2), \tag{6.11}$$

$$\phi^4(y_1,y_2) = \cos(\pi y_2)\sin(2\pi y_1). \tag{6.12}$$

Next, we calculate

$$\phi^1_{,1}(y_1,y_2) = \begin{cases} -(1-\xi) & \text{if} \quad y_1 \in \left(-\dfrac{\xi}{2}, \dfrac{\xi}{2}\right), \\ \xi & \text{if} \quad y_1 \in \left(\dfrac{-1}{2}, -\dfrac{\xi}{2}\right) \cup \left(\dfrac{\xi}{2}, \dfrac{1}{2}\right); \end{cases} \tag{6.13}$$

$$\phi^1_{,2}(y_1,y_2) = 0, \qquad \phi^2_{,1}(y_1,y_2) = 0; \tag{6.14}$$

$$\phi^2_{,2}(y_1,y_2) = \begin{cases} -(1-\xi) & \text{if} \quad y_2 \in \left(-\dfrac{\xi}{2}, \dfrac{\xi}{2}\right), \\ \xi & \text{if} \quad y_2 \in \left(-\dfrac{1}{2}, -\dfrac{\xi}{2}\right) \cup \left(\dfrac{\xi}{2}, \dfrac{1}{2}\right); \end{cases} \tag{6.15}$$

$$\begin{aligned} \phi^3_{,1}(y_1,y_2) &= -\pi\sin(\pi y_1)\sin(2\pi y_2), \\ \phi^3_{,2}(y_1,y_2) &= 2\pi\cos(\pi y_1)\cos(2\pi y_2); \end{aligned} \tag{6.16}$$

$$\begin{aligned} \phi^4_{,1}(y_1,y_2) &= 2\pi\cos(2\pi y_1)\cos(\pi y_2), \\ \phi^4_{,2}(y_1,y_2) &= -\pi\sin(2\pi y_1)\sin(\pi y_2). \end{aligned} \tag{6.17}$$

Substituting (6.13)–(6.17) into (6.8), from (6.4) we can determine the dependence of the approximate value of the effective conductivity coefficient λ_e on the macroscopic temperature T. To find such a dependence it has been assumed that

$$\theta = \frac{|Y_1|}{|Y|} = \xi^2 = 0.75,$$

while the conductivity coefficients of the phases are given by:

a) (see Fig. 5) $\lambda_1 = 0.21 + 0.005T, \quad \lambda_2 = 37.25 + 0.048T,$

b) (see Fig. 6) $\lambda_1 = 37.25 + 0.048T, \quad \lambda_2 = 0.21 + 0.005T.$

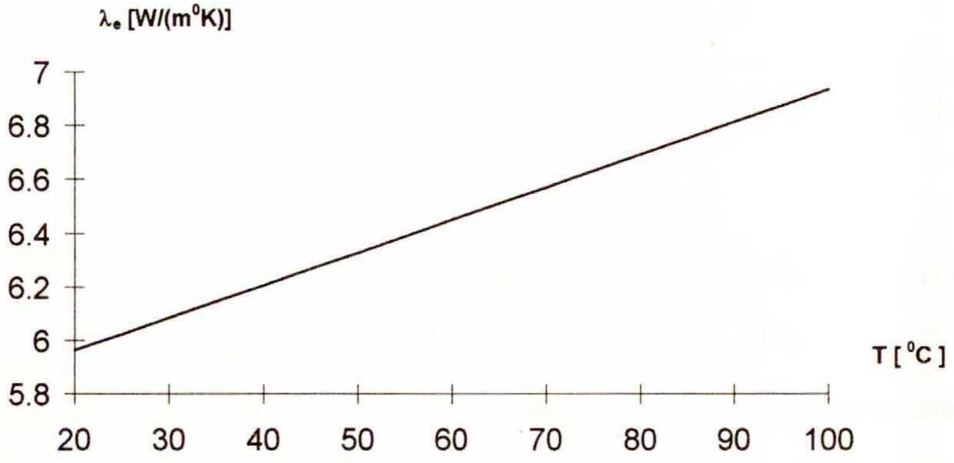

FIG. 5. The effective conductivity versus temperature; in the inclusion: $\lambda_1 = 0.21 + 0.005T$, in the matrix: $\lambda_2 = 37.25 + 0.048T$, volume ratio: $\theta = 0.75$.

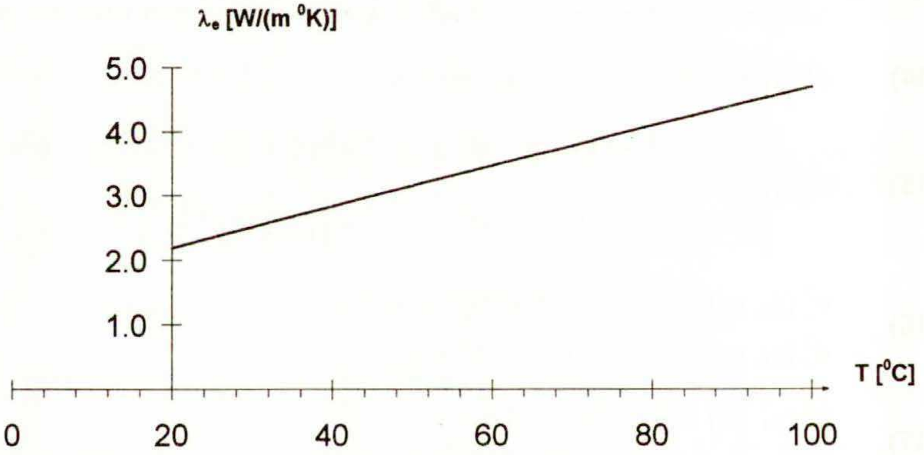

FIG. 6. The effective conductivity versus temperature; in the inclusion: $\lambda_1 = 37.25 + 0.048T$, in the matrix: $\lambda_2 = 0.21 + 0.005T$, volume ratio: $\theta = 0.75$.

7. Bounds on the effective conductivity of two-phase composites. Padé approximants method

In this section we shall use the formulae for finding bounds on the effective heat conductivity $\lambda_e(\eta(T))$ by assuming that at the macroscopic scale the composite is isotropic. Towards this end the method of Padé approximants is applied. The same procedure can also be used for the determination of bounds on the diagonal elements of the effective conductivity matrix, what follows from Theorem 2. For macroscopically isotropic materials the Stieltjes integral representation of the effective conductivity $\lambda_e(\eta(T))/\lambda_2(T)$ is given by, cf. (4.11),

$$\frac{\lambda_e(\eta(T))}{\lambda_2(T)} - 1 = \eta(T)f_1(\eta(T)) = \eta(T)\int\limits_0^1 \frac{d\gamma_1(z)}{1+\eta(T)z}, \quad 0 \le z \le 1. \tag{7.1}$$

Moreover the following inequality is satisfied, cf. [19]

$$\lim_{\eta(T)\to -1^+} \eta(T)f_1(\eta(T)) \ge -1. \tag{7.2}$$

Consider the power expansion of $\eta(T)f_1(\eta(T))$ at $\eta(T)=0$:

$$\eta(T)f_1(\eta(T)) = \sum_{n=1}^{\infty} c_n \eta^n(T), \tag{7.3}$$

where

$$c_n = (-1)^{n+1}\int\limits_0^1 z^{n-1} d\gamma_1(z). \tag{7.4}$$

The one-point Padé approximants $[p/M']$ and $[p/M'']$ to the effective conductivity $\lambda_e(\eta(T))/\lambda_2(T)$ represented by $\eta(T)f_1(\eta(T))$ are given by:

$$[p/M'] = \frac{a'_1\eta(T) + a'_2\eta^2(T) + \cdots + a'_{M'}\eta^{p-M'}(T)}{1 + b'_1\eta(T) + b'_2\eta^2(T) + \cdots + b'_{M'}\eta^{M'}(T)}, \quad M' = E(p/2), \tag{7.5}$$

$$[p/M''] = \frac{a''_1\eta(T) + a''_2\eta^2(T) + \cdots + a''_{M''}\eta^{p+1-M''}(T)}{1 + b''_1\eta(T) + b''_2\eta^2(T) + \cdots + b''_{M''}\eta^{M''}(T)}, \quad M'' = E((p+1)/2). \tag{7.6}$$

Here $E(w)$ is the entier function, i.e. the greatest natural number not exceeding w. Observe that now $[p/M']$ and $[p/M'']$ depend on the macroscopic temperature T.

Consider the power expansions of $[p/M']$ and $[p/M'']$ at $\eta(T)=0$:

$$[p/M'] = \sum_{n=1}^{\infty} c'_n \eta^n(T), \qquad [p/M''] = \sum_{n=1}^{\infty} c''_n \eta^n(T). \tag{7.7}$$

DEFINITION 1. *The rational functions* (7.5), (7.6) *are the one-point Padé approximants to the Stieltjes function* (7.1):

(i) *of the type* $[p/M']$, $M' = E(p/2)$, *if*

$$c'_n = c_n^{(1)} \qquad \text{for } n = 1, 2, \ldots, p; \tag{7.8}$$

(ii) *of the type* $[p/M'']$, $M'' = E((p+1)/2)$, *if*

$$(7.9) \qquad c''_n = c^{(1)}_n \quad \text{for } n = 1, 2, \ldots, p, \qquad [p/M''] = -1 \quad \text{for } \eta(T) = -1. \ \square$$

The parameter p *appearing in this definition denotes a number of available coefficients of the power series* (7.3) *matched by Padé approximants* $[p/M']$ *and* $[p/M'']$.

Let us recall the basic results of the paper [38].

THEOREM 3. *The one-point Padé approximants* $[p/M']$ *and* $[p/M'']$ *satisfy the following inequalities:*

(i) *If* $-1 < \eta(T) < 0$ *then*

$$(7.10) \qquad [p/M'] > [p+1/M'],$$

$$(7.11) \qquad [p/M''] < [p+1/M''],$$

$$(7.12) \qquad [p/M'] \geq \eta(T) f_1(\eta(T)) \geq [p/M''].$$

(ii) *If* $0 < \eta(T) < \infty$ *then*

$$(7.13) \qquad (-1)^p[p/M'] < (-1)^p[p+2/M'],$$

$$(7.14) \qquad (-1)^p[p/M''] > (-1)^p[p+2/M''],$$

$$(7.15) \qquad (-1)^p[p/M'] \leq (-1)^p \eta(T) f_1(\eta(T)) \leq (-1)^p[p/M''].$$

Moreover

$$\eta(T) f_1(\eta(T)) = \lim_{p\to\infty} [p/M'] = \lim_{p\to\infty} [p/M''].$$

The inequalities (7.10) – (7.12) *and* (7.13) – (7.15) *have the consequence that Padé approximants* $[p/M']$ *and* $[p/M'']$ *form the best upper and lower bounds on* $\eta(T) f_1(\eta(T))$ *obtainable using only* p *coefficients of a series* (7.3), *and that the use of additional coefficients (higher* p*) improves the bounds.* $\square$

It is convenient to represent the Padé approximants $[p/M']$ and $[p/M'']$ by S-continued fractions, cf. [36],

$$(7.16) \qquad [p/M'] = \frac{g_1\eta(T)}{1} \, {}_{+} \, \frac{g_2\eta(T)}{1} \, {}_{+} \cdots {}_{+} \, \frac{g_{p-2}\eta(T)}{1} \, {}_{+} \, \frac{g_{p-1}\eta(T)}{1} \, {}_{+} \, \frac{g_p\eta(T)}{1},$$

$$(7.17) \qquad [p/M''] = \frac{g_1\eta(T)}{1} \, {}_{+} \, \frac{g_2\eta(T)}{1} \, {}_{+} \cdots {}_{+} \, \frac{g_{p-1}\eta(T)}{1} \, {}_{+} \, \frac{g_p\eta(T)}{1} \, {}_{+} \, \frac{V_{p+1}\eta(T)}{1},$$

where

$$\frac{g_1\eta(T)}{1} \, {}_{+} \, \frac{g_2\eta(T)}{1} \, {}_{+} \cdots {}_{+} = \frac{g_1\eta(T)}{1 + \dfrac{g_2\eta(T)}{1 + \cdots}}.$$

The coefficients g_m $(m = 1, 2, \ldots, p)$ are determined by the following recurrence relations

$$(7.18) \qquad \left\{ \begin{array}{l} \qquad\qquad m = 1, 2, \ldots, p, \quad g_m = c_1^{(m)}, \\ \left\{ \begin{array}{l} n = 1, 2, \ldots, p - m, \\ c_0^{(1+m)} = 1, \quad c_n^{(1+m)} = -\dfrac{1}{c_1^{(m)}} \left\{ \displaystyle\sum_{j=0}^{n-1} c_j c_{n+1-j}^{(m)} \right\}, \end{array} \right. \end{array} \right.$$

with input data c_m $(m = 1, 2, \ldots, p)$ given by (7.3), cf. [41]. Also a simple recurrence formulae determine the coefficients V_{p+1}

$$(7.19) \qquad V_1 = 1, \qquad V_{1+j} = \frac{V_j - g_j}{V_j}, \quad j = 1, 2, \ldots, p$$

and the Padé approximants $[p/M']$ ($[p/M'']$)

$$Q^{(0)} = V_{p+1} = 0 \quad \text{for} \quad [p/M'], \qquad (Q^{(0)} = \eta(T)V_{p+1} \quad \text{for} \quad [p/M'']),$$

$$(7.20) \qquad Q^{(j+1)} = \frac{\eta(T)g_{p-j}}{1 + Q^{(j)}}, \qquad j = 0, 1, \ldots, p - 1,$$

$$[p/M'] = Q^{(p)}, \qquad ([p/M'] = Q^{(p)}).$$

Relations (7.18) – (7.20) allow us to compute Padé approximants bounds on $\lambda_e(\eta(T))/\lambda_2(T)$ in terms of $[p/M']$ and $[p/M'']$, from power expansion given by (7.3).

Let us pass now to an application of the Padé approximants method for the determination of the nonlinear effective conductivity $\lambda_e(T)$ of a composite, which consists of the regularly spaced and equally-sized cylinders of the conductivity $\lambda_2(T)$ embedded in a matrix material of the conductivity $\lambda_1(T)$. We set: $\theta = \pi\rho^2$-volume fraction, ρ-radius of cylinders, $\eta(T) = (\lambda_1(T)/\lambda_2(T)) - 1$-nondimensional conductivity. The input data for determining the Padé bounds given by power series, cf. (7.3),

$$(7.21) \qquad \eta(T)f_1(\eta(T)) = \sum_{n=1}^{\infty} (\pi d_1^{(n)} \rho^2) \eta^n(T), \qquad c_n = \pi d_1^{(n)} \rho^2,$$

have been computed by means of the recurrence formulae derived in [39]:

$$(7.22) \qquad d_m^{n+1} = -\sum_{k=1}^{\infty} d_k^n \left(\frac{1}{2}\delta_{mk} + a_{km} \frac{m\rho^{k+m}}{2k!} \right), \qquad d_m^{(1)} = \delta_{m1},$$

$$(7.23) \qquad a_{km} = (-1)^k \frac{(m+k)!}{m!} \left(A_{km} + \frac{1}{2}\pi\delta_{(m+k)2} \right), \quad \delta_{mk} = \left\{ \begin{array}{ll} 1, & \text{if } m = k, \\ 0, & \text{if } m \neq k. \end{array} \right.$$

Here A_{km} are the coefficients of the Wigner potential evaluated in [42, 43]. The low order Padé bounds $[p/M']$ and $[p/M'']$ on $\lambda_e(\eta(T))/\lambda_2(T)$ of a square array of cylinders are depicted in Fig. 7. According to (4.11) the obtained bounds are universal, i.e., they are valid for arbitrary, continuous functions $\lambda_2(T)$ and $\lambda_1(T)$. From those universal bounds one can pass to bounds on λ_e as a function of T, cf. Figs. 8, 9.

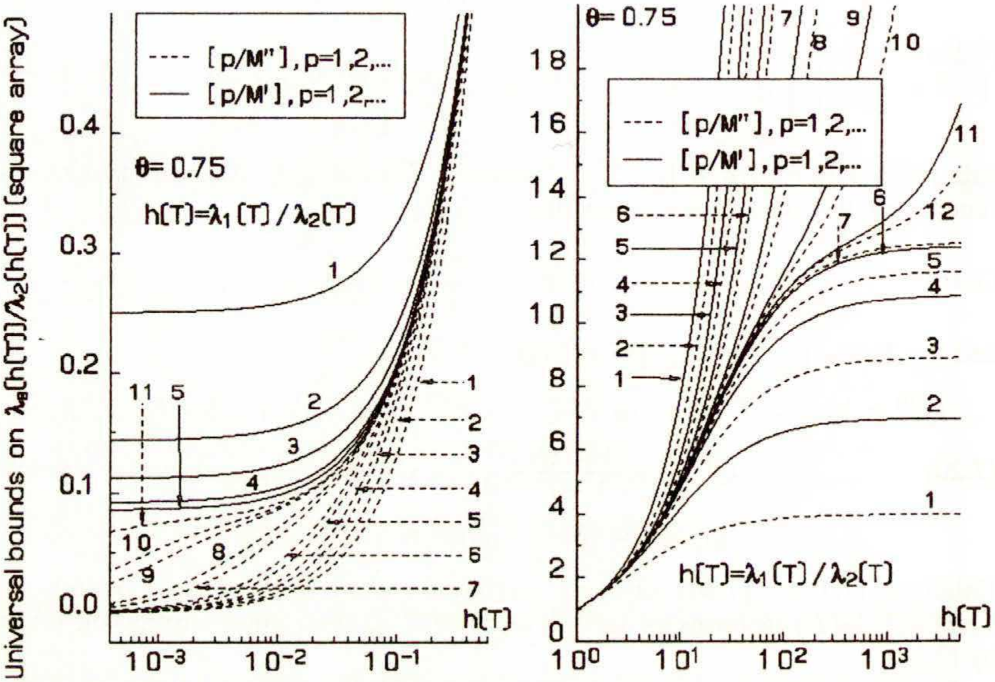

FIG. 7. Sequences of Padé approximants forming upper and lower bounds on the effective conductivity of a square array of cylinders.

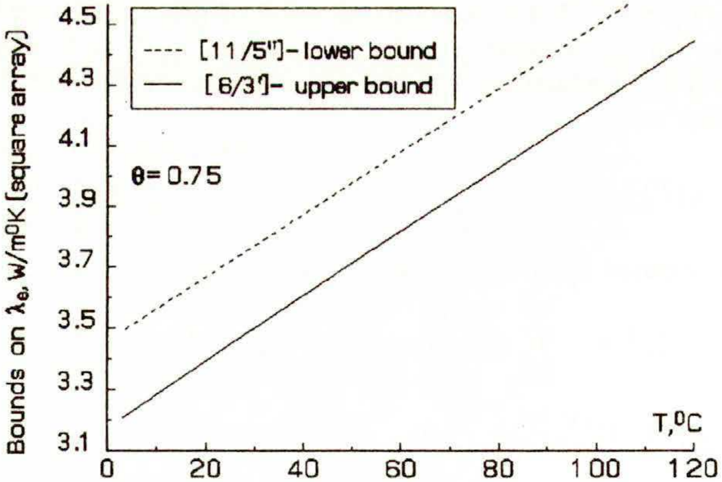

FIG. 8. Upper and lower bounds on the effective conductivity for square array of cylinders (epidian 53, $\lambda_1 = 0.21 + 0.005T$), embedded in a matrix (steel 15NiCuMoNb5, $\lambda_2 = 37.25 + 0.048T$), cf. [44].

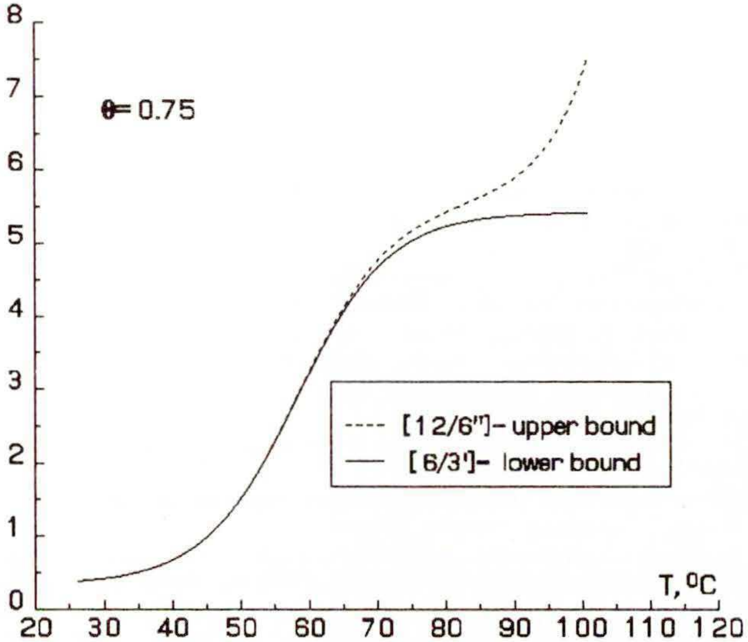

FIG. 9. Upper and lower bounds on the effective conductivity of human tissues: bones with $\lambda_1 = 0.349$ and muscles with $\lambda_2 = 0.29 + 0.29\exp((0.15(T - 36.7))$, cf. [29].

To illustrate the above procedure we have evaluated the effective conductivity λ_e versus temperature T for the composite consisting of the steel 15NiCuMoNb5 with $\lambda_1 = 37.25 + 0.048T$ and epidian 53 with $\lambda_2 = 0.21 + 0.005T$, cf. Fig. 8. The next example deals with live tissues: bone with $\lambda_2 = 0.436$ and muscles with $\lambda_1 = 0.29 + 0.29\exp 0.15(T - 36.7)$, cf. Fig. 9. All conductivities are given in [W/m°K].

Acknowledgment

This work was supported by the State Committee for Scientific Research (Poland) through the grant No. 3 P404 013 06.

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Received November 7, 1996.