Arch. Mech., **49**, 4, pp. 647–663, Warszawa 1997

Rigorous bounds on the asymptotic expansions of effective transport coefficients of two-phase media

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THE FUNDAMENTAL inequalities for two-point Padé approximants corresponding to two asymptotic expansions of the effective transport coefficients $\lambda_e(x)/\lambda_1$, $x = \lambda_2/\lambda_1 - 1$ have been derived, where λ_1 and λ_2 denote the transport moduli of the composite components. The inequalities achieved constitute the new bounds on the values of $\lambda_e(x)/\lambda_1$ – the best with respect to the given number of coefficients of the asymptotic expansions of $\lambda_e(x)/\lambda_1$ at $x = 0$ and $x = \infty$. For the particular cases, our two-point Padé bounds reduce to the classical estimations of $\lambda_e(x)/\lambda_1$ available in literature [7, 9, 17, 24].

1. Introduction

PREDICTION of the macroscopic behaviour of a composite from the known physical and geometrical properties of the components is one of the basic problems of mechanics of inhomogeneous media. Most of the papers which have appeared in recent years dealt with the estimations of the effective transport coefficients $\lambda_e(x)$, $x = \lambda_2/\lambda_1 - 1$ such as thermal and electrical conductivities, magnetic permeability, diffusion coefficient, filtration coefficients and many others. Here λ_1 and λ_2 denote the moduli of the components of an investigated composite, cf. [6, 7, 9, 17, 23, 24].

WIENER [34] derived optimal bounds on $\lambda_e(x)$ with prescribed volume fractions. These bounds are known as the arithmetic and harmonic mean bounds. For isotropic materials HASHIN and SHTRIKMAN [17] improved Wiener's bounds using variational principles. BERGMAN [4, 5, 6] introduced a method for obtaining bounds on $\lambda_e(x)$, which does not rely on variational principles. Instead it exploits the properties of the effective parameters being analytic functions of the components moduli. The method of Bergman was studied in more detail and applied to several physical problems by MILTON [23, 24]. A rigorous justification of Bergman's approach was given by GOLDEN and PAPANICOLAOU [14]. Recently special continued fraction techniques for evaluation of the bounds on $\lambda_e(x)$ have been used by BERGMAN [7] for three-dimensional, and CLARK and MILTON [9] – for two-dimensional systems. Both MILTON [24] and BERGMAN [7] have incorporated into the bounds the power expansion of $\lambda_e(x)$ at $x = 0$ and the discrete values of $\lambda_e(x)$ given by $\lambda_e(x_1)$, $\lambda_e(x_2)$, ..., $\lambda_e(x_K)$ only.

The present paper incorporates into bounds on $\lambda_e(x)$ two formal power expansions of $\lambda_e(x)$ available at $x = 0$ and $x = \infty$. That incorporation problem has been studied recently in the contexts of the estimation of Stieltjes functions [11, 25, 27, 28] and the bounds on the effective conductivity of regular composites [26, 29 – 32]. However, the estimations derived in [11, 28, 29] are valid for $x > 0$ only. Consequently they are not the best possible bounds on $\lambda_e(x)$.

The main aim of this paper is to establish new bounds on real-valued moduli $\lambda_e(x)$ of two-phase media, the best with respect to the available coefficients of the power expansions of $\lambda_e(x)$ at $x = 0$ and $x = \infty$.

This paper is organized as follows: In Sec. 2 we introduce the basic definitions, notations and assumptions dealing with a Stieltjes function $xf_1(x)$ and two-point Padé approximants of the types $2PAs$ and $\overline{2PAs}$ constructed for $xf_1(x)$. In Sec. 3 we recall the relevant results for one-point Padé approximants. In Sec. 4 we propose special continued fraction representations for $2PAs$ and $\overline{2PAs}$. The fundamental inequalities for $2PAs$ and $\overline{2PAs}$ to $xf_1(x)$ have been derived in Sec. 5 and 6. In Sec. 7 the effective conductivity of a square array of cylinders has been investigated in terms of low order $2PAs$ and $\overline{2PAs}$ bounds. The results achieved are summarized in Sec. 8.

2. Preliminaries

Let us consider the effective conductivity $\Lambda_e(x)$ of a two-phase medium for the case, where the conductivity coefficients λ_1 and λ_2 of both components are real, $x = (\lambda_2/\lambda_1) - 1$. The bulk conductivity $\Lambda_e(x)$ is defined by the linear relationship between the volume-averaged gradient temperature $<\overrightarrow{\nabla T}>$ and the volume-averaged heat flux $< \vec{q} >$

$$< \vec{q} >= \Lambda_e(x) <\overrightarrow{\nabla T}> . \tag{2.1}$$

For the sake of simplicity, the averaging is performed over the unit cell of a periodic composite, where T denotes the temperature. In general, Λ_e is a second-rank symmetric tensor, even when λ_1 and λ_2 are both scalars. Our study will be focused upon one of the diagonal values of Λ_e denoted by λ_e. The remaining diagonals can be studied analogously.

The analytic properties of the bulk conductivity coefficient $\lambda_e(\lambda_1, \lambda_2)$ were examined by BERGMAN in [4]. He noticed that $\lambda_e(\lambda_1, \lambda_2)/\lambda_1 = \lambda_e(1, \lambda_2/\lambda_1)$ is an analytical function in the complex plane except on the negative part of the real axis. GOLDEN and PAPANICOLAOU [14] rigorously proved that $\lambda_e(x)$, $x = h - 1$, $h = \lambda_2/\lambda_1$ has a Stieltjes-integral representation of the type:

$$\frac{\lambda_e(x)}{\lambda_1} - 1 = xf_1(x) = x\int_0^1 \frac{d\gamma_1(u)}{1 + xu}, \qquad -1 < x < \infty. \tag{2.2}$$

For composites consisting of non-touching inclusions of modulus λ_2 embedded in a matrix material of modulus λ_1, the function $xf_1(x)$ obeys the following physical restriction, cf. [4 – 7],

$$\lim_{x\to -1_+} xf_1(x) \geq -1. \tag{2.3}$$

The spectrum $\gamma_1(u)$ appearing in (2.2) is a real, bounded and non-decreasing function defined on $0 \leq u \leq 1$. Consider the power expansion of $xf_1(x)$ at $x = 0$, cf. (2.2),

$$xf_1(x) = \sum_{n=1}^{\infty} c_n^{(1)} x^n. \tag{2.4}$$

Here the coefficients

$$c_n^{(1)} = (-1)^{n+1} \int_0^1 u^{n-1}\, d\gamma_1(u) \tag{2.5}$$

are real and finite. Note that on account of (2.2), the power series (2.4) has a radius of convergence at least equal 1. The power series expansion of $xf_1(x)$ at $x = \infty$ takes the form, cf. (2.2),

$$xf_1(x) = \sum_{n=0}^{\infty} C_n^{(1)} s^n, \qquad s = 1/x, \tag{2.6}$$

where the moments

$$C_n^{(1)} = (-1)^n \int_0^1 u^{-1-n}\, d\gamma_1(u), \qquad n = 0, 1, 2, \ldots \tag{2.7}$$

are assumed to be finite for any fixed n. Two-point Padé approximants of the type $[k/M]$ and $\overline{[k/M]}$ to series (2.4) and (2.6) are given by the following rational functions

$$[k/M] = \frac{a_{1k}x + a_{2k}x^2 + \cdots + a_{Mk}x^M}{1 + b_{1k}x + b_{2k}x^2 + \cdots + b_{Mk}x^M}, \tag{2.8}$$

$$\overline{[k/M]} = \frac{\overline{a}_{1k}x + \cdots + \overline{a}_{(M+\delta_{0k})k}x^{(M+\delta_{0k})}}{1 + \overline{b}_{1k}x + \cdots + \overline{b}_{Mk}x^M}, \qquad \delta_{0k} = \begin{cases} 1, & \text{if } k = 0, \\ 0, & \text{if } k > 0. \end{cases} \tag{2.9}$$

Consider the power expansions of (2.8) and (2.9) at $x = 0$:

$$[k/M] = \sum_{n=1}^{\infty} c_{nk} x^n, \qquad \overline{[k/M]} = \sum_{n=1}^{\infty} \overline{c}_{nk} x^n, \tag{2.10}$$

and at $x = \infty$

$$(2.11) \qquad [k/M] = \sum_{n=0}^{\infty} C_{nk} s^n, \qquad \overline{[k/M]} = \sum_{n=0}^{\infty} \overline{C}_{nk} s^n, \qquad s = 1/x.$$

Now we are in a position to introduce the definitions of two-point Padé approximants of the types $2PAs$ and $\overline{2PAs}$ to $xf_1(x)$:

DEFINITION 1. *The rational function* $[k/M]$ *given by* (2.8) *is a* $2PAs$ *(two-point Padé approximant) to* $xf_1(x)$, *if*

$$(2.12) \qquad c_{nk} = c_n^{(1)} \qquad \textit{for} \quad n = 1, 2, ..., p, \quad p = 2M - k$$

and

$$(2.13) \qquad C_{nk} = C_n^{(1)} \qquad \textit{for} \quad n = 0, 1, ..., k-2, \quad C_{(k-1)k} = C_{k-1}^{(1)}.$$

Note that for $k = 0$ *and* $k = 2M$, *the rational functions* $[k/M]$ *stand for one-point Padé approximants* ($1PAs$), cf. [1, 2]. □

DEFINITION 2. *The rational function* $\overline{[k/M]}$ *given by* (2.9) *is a* $\overline{2PAs}$ *to* $xf_1(x)$, *if*

$$(2.14) \qquad \overline{c}_{nk} = c_n^{(1)} \qquad \textit{for} \quad n = 1, 2, ..., p, \quad p = 2M - k,$$

and

$$(2.15) \qquad \begin{aligned} \overline{C}_{nk} &= C_n^{(1)} && \textit{for} \quad n = 0, 1, ..., k-2, \\ \overline{[k/M]} &= -1 && \textit{for} \quad x = -1. \end{aligned} \quad \square$$

Throughout this paper the parameter p $(0 \leq p \leq 2M)$ will denote a number of the available coefficients of the power series (2.4), while k $(0 \leq k \leq 2M)$ – a number of relations given by (2.13) if we deal with $[k/M]$, or by (2.15) if we study $\overline{[k/M]}$. The parameters p, k and M are interrelated by $p + k = 2M$.

3. One-point Padé approximants

We start our discussion by recalling some results for one-point Padé approximants $[0/M]$ to $xf_1(x)$, indispensable for our further investigations. Those results may be summarized as follows:

1. $[0/M]$ has the continued fraction representation of the type S [1–3]

$$(3.1) \qquad [0/M] = \frac{xe_1}{1} + \frac{xe_2}{1} + \ldots + \frac{xe_{2M-1}}{1} + \frac{xe_{2M}}{1}.$$

2. The coefficients of the continued fraction (3.1) are positive

$$e_n > 0, \qquad n = 1, 2, \ldots, 2M. \tag{3.2}$$

3. For $x > -1$ the Padé approximants $[0/M]$ to power series (2.4) converge to the Stieltjes function (2.2), cf. [1, Th. 16.2]

$$\lim_{M\to\infty} [0/M] = x f_1(x). \tag{3.3}$$

4. If $x f_j(x)$ is a Stieltjes function

$$x f_j(x) = x \int_0^1 \frac{d\gamma_j(u)}{1 + xu}, \tag{3.4}$$

then the function $x f_{j+1}(x)$ is also a Stieltjes function

$$x f_{j+1}(x) = x \int_0^1 \frac{d\gamma_{j+1}(u)}{1 + xu}, \tag{3.5}$$

provided that

$$f_j(x) = \frac{f_j(0)}{1 + x f_{j+1}(x)}, \tag{3.6}$$

cf. [1, Lemma 15.3] and [1, p. 235]. If the expansion of $x f_j(x)$ at $x = \infty$ is given by

$$x f_j(x) = \sum_{n=0}^{\infty} C_n^{(j)} (1/x)^n, \qquad C_0^{(j)} > 0, \tag{3.7}$$

then on account of (3.6), the expansion of $x f_{j+1}(x)$, also at $x = \infty$, takes the form

$$x f_{j+1}(x) = C^{(j+1)} x + \sum_{n=0}^{\infty} C_n^{(j+2)} (1/x)^n, \qquad C^{(j+1)} = \frac{f_j(0)}{C_0^{(j)}} > 0. \tag{3.8}$$

Consequently we have the following relations

$$x f_{j+1}(x) = C^{(j+1)} x + x f_{j+2}(x), \tag{3.9}$$

where

$$f_{j+2}(x) = \int_0^1 \frac{d\gamma_{j+2}(u)}{1 + xu} \tag{3.10}$$

is a Stieltjes function. The relations (3.7) – (3.10) permit us to formulate the following remark:

REMARK 1. If $xf_j(x)$ is a Stieltjes function

$$xf_j(x) = x\int_0^1 \frac{d\gamma_j(u)}{1+xu} = \sum_{n=0}^{\infty} C_n^{(j)} s^n, \qquad s = 1/x, \tag{3.11}$$

then $xf_{j+2}(x)$ is also a Stieltjes function

$$xf_{j+2}(x) = x\int_0^1 \frac{d\gamma_{j+2}(u)}{1+xu}, \tag{3.12}$$

provided that

$$f_j(x) = \frac{f_j(0)}{1 + C^{(j+1)}x + xf_{j+2}(x)}, \qquad C^{(j+1)} = \frac{f_j(0)}{C_0^{(j)}}. \qquad \square \tag{3.13}$$

Note that by inserting $x = 1/s$ into (3.4) we obtain the identity

$$xf_j(x) = s^{-1}\int_0^1 \frac{d\gamma_j(u)}{s+u} = \varphi_j(s) = \int_1^{\infty} \frac{d\beta_j(\tau)}{1+s\tau}, \tag{3.14}$$

where

$$d\beta_j(\tau) = -\frac{1}{\tau} d\gamma_j(1/\tau) \geq 0. \tag{3.15}$$

REMARK 2. If $xf_j(x)$ is a Stieltjes function with respect to a variable x, then $\varphi_j(s) = xf_j(x)$ is a Stieltjes function with respect to s, provided $x = 1/s$, cf. (3.14) – (3.15). □

The fractional transformations (3.6) and (3.13) and the identity (3.14) will be used for the construction of a special continued fraction representations for Padé approximants $[k/M]$ and $\overline{[k/M]}$, cf. (2.8) – (2.15).

4. Continued fractions for $2PAs$ and $\overline{2PAs}$

Let us apply the fractional transformation (3.13) to $xf_1(x)$ k times. Thus we obtain a T-continued fraction to $xf_1(x)$, cf. [15, 20],

$$xf_1(x) = \frac{xG_1}{1+xG_2} \, {}_{+} \, \frac{xG_3}{1+xG_4} \, {}_{+} \, \ldots \, {}_{+} \, \frac{xG_{2k-1}}{1+xG_{2k}+xf_{2k+1}(x)}. \tag{4.1}$$

Here the parameters G_n are uniquely determined by the initial k coefficients of a power series (2.4) and (2.6). On account of Remark 2, for $s = 1/x$ we have $xf_{2k+1}(x) = \varphi_{2k+1}(s)$, where $xf_{2k+1}(x)$ and $\varphi_{2k+1}(s)$ are Stieltjes functions. By employing the transformation (3.6) $(p-k)$ times to the function $xf_{2k+1}(x)$, if $p > k$ and $(k-p)$ times to $\varphi_{2k+1}(s)$, if $k > p$ we arrive at

$$(4.2)\qquad xf_{2k+1}(x) = \begin{cases} \dfrac{xg_{2k+1}}{1} \underset{+}{} \dfrac{xg_{2k+2}}{1} \underset{+}{} \ldots \underset{+}{} \dfrac{xg_{p+k}}{1 + xf_{p+k+1}(x)}, & p \geq k, \\[2ex] \dfrac{d_{2p+1}}{1} \underset{+}{} \dfrac{d_{2p+2}}{x} \underset{+}{} \dfrac{d_{2p+3}}{1} \underset{+}{} \ldots \underset{+}{} \dfrac{d_{p+k}}{x + xt_{p+k+1}(x)}, & k \geq p. \end{cases}$$

Note that functions $f_{p+k+1}(x)$ and $t_{p+k+1}(x)$ appearing in (4.2) are also Stieltjes functions of the type (2.2). The substitution of (4.2) into (4.1) yields the continued fraction representations for Padé approximants $[k/M]$, $[2M-p/M]$

$$(4.3)\qquad \begin{aligned} [k/M] &= \frac{xG_1}{1+xG_2} \underset{+}{} \cdots \underset{+}{} \frac{xG_{2k-1}}{1+xG_{2k}} \underset{+}{} \frac{xg_{2k+1}}{1} \underset{+}{} \ldots \underset{+}{} \frac{xg_{2M}}{1}, \\ [2M-p/M] &= \frac{xG_1}{1+xG_2} \underset{+}{} \cdots \underset{+}{} \frac{xG_{2p-1}}{1+xG_{2p}} \underset{+}{} \frac{d_{2p+1}}{1} \underset{+}{} \frac{d_{2p+2}}{x} \\ &\quad \underset{+}{} \frac{d_{2p+3}}{1} \underset{+}{} \ldots \underset{+}{} \frac{d_{2M}}{x}, \end{aligned}$$

and $\overline{[k/M]}$, $\overline{[2M-p/M]}$

$$(4.4)\qquad \begin{aligned} \overline{[k/M]} &= \frac{xG_1}{1+xG_2} \underset{+}{} \cdots \underset{+}{} \frac{xG_{2k-1}}{1+xG_{2k}} \underset{+}{} \frac{xg_{2k+1}}{1} \\ &\quad \underset{+}{} \ldots \underset{+}{} \frac{xg_{2M}}{1} \underset{+}{} \frac{xV_{2M+1}}{1}, \\ \overline{[2M-p/M]} &= \frac{xG_1}{1+xG_2} \underset{+}{} \cdots \underset{+}{} \frac{xG_{2p-1}}{1+xG_{2p}} \underset{+}{} \frac{d_{2p+1}}{1} \underset{+}{} \frac{d_{2p+2}}{x} \\ &\quad \underset{+}{} \ldots \underset{+}{} \frac{d_{2M}}{x} \underset{+}{} \frac{xT_{2M+1}}{1}. \end{aligned}$$

On account of Def. 2, V_{2M+1} and T_{2M+1} satisfy the relations

$$(4.5)\qquad \begin{aligned} &\frac{xG_1}{1+xG_2} \underset{+}{} \cdots \underset{+}{} \frac{xG_{2k-1}}{1+xG_{2k}} \underset{+}{} \frac{xg_{2k+1}}{1} \underset{+}{} \ldots \underset{+}{} \frac{xg_{2M}}{1} \\ &\quad \underset{+}{} \frac{xV_{2M+1}}{1} = -1, \qquad \text{if} \quad x = -1, \\ &\frac{xG_1}{1+xG_2} \underset{+}{} \cdots \underset{+}{} \frac{xG_{2p-1}}{1+xG_{2p}} \underset{+}{} \frac{d_{2p+1}}{1} \underset{+}{} \frac{d_{2p+2}}{x} \underset{+}{} \ldots \underset{+}{} \frac{d_{2M}}{x} \\ &\quad \underset{+}{} \frac{xT_{2M+1}}{1} = -1, \qquad \text{if} \quad x = -1. \end{aligned}$$

For $k > 0$ the parameters p, k, M are interrelated by

$$p + k = 2M, \qquad 0 < k < 2M, \qquad 0 < p < 2M. \tag{4.6}$$

The coefficients G_n $(n = 1, 2, ..., 2k)$, g_{2k+j} $(j = 1, 2, ..., p - k)$, V_{2M+1}, d_{2k+j} $(j = 1, 2, ..., k - p)$ and T_{2M+1} appearing in (4.3) – (4.4) are positive, i.e.,

$$\begin{aligned} &G_n > 0, && n = 1, 2, ..., 2k; && \\ &g_{2k+j} > 0, && j = 1, 2, ..., p - k \geq 0; && V_{2M+1} > 0, \\ &G_n > 0, && n = 1, 2, ..., 2p; && \\ &d_{2k+j} > 0, && j = 1, 2, ..., k - p \geq 0; && T_{2M+1} > 0. \end{aligned} \tag{4.7}$$

Now we are in a position to study the convergence of $[k/M]$ (k fixed) and $[2M - p/M]$ (p fixed) to $xf_1(x)$, when M goes to infinity. Due to nonzero radius of convergence of the power expansion (4.2) we infer, cf. [2, Th. 16.2],

$$\begin{aligned} &\lim_{M\to\infty} \frac{xg_{2k+1}}{1} + \frac{xg_{2k+2}}{1} + \ldots + \frac{xg_{2M}}{1} = xf_{2k+1}(x), \quad -1 < x < \infty, \\ &\lim_{M\to\infty} \frac{d_{2p+1}}{1} + \frac{d_{2p+2}}{x} + \frac{d_{2p+3}}{1} + \ldots + \frac{d_{2M}}{x} = xf_{2k+1}(x), \quad -1 < x < \infty. \end{aligned} \tag{4.8}$$

Consequently the relation (4.1) yields

$$\lim_{M\to\infty} [k/M] = \lim_{M\to\infty} [2M - p/M] = xf_1(x), \qquad -1 < x < \infty. \tag{4.9}$$

From (4.3) and (4.4), it follows: $\overline{[k/M]} = [k/M]$, if $V_{2M+1} = 0$; $\overline{[k/M]} = [k - 1/M - 1]$, if $V_{2M+1} = \infty$; $\overline{[2M - p/M]} = [2M - p/M]$, if $T_{2M+1} = 0$; $\overline{[2M - p/M]} = [2M - p - 1/M - 1]_{2M-p-1}$, if $T_{2M+1} = \infty$. For $x \in (0, \infty)$ $\overline{[k/M]}$ and $\overline{[2M - p/M]}$ are monotonic functions of the parameters $V_{2M+1} \geq 0$ and $T_{2M+1} \geq 0$, respectively. Hence for fixed $x \in (0, \infty)$, $\overline{[k/M]}$ takes values within $[k/M]$ and $[k - 1/M - 1]$, while $\overline{[2M - p/M]}$ within $[2M - p/M]$ and $[2M - p - 1/M - 1]$. On account of that and due to (4.9) we obtain

$$\lim_{M\to\infty} \overline{[k/M]} = \lim_{M\to\infty} \overline{[2M - p/M]} = xf_1(x), \qquad 0 < x < \infty. \tag{4.10}$$

The Padé approximants $\overline{[k/M]}$ and $\overline{[2M - p/M]}$ are analytical functions for $-1 < x < \infty$ (their poles lie on the real axis at $-\infty < x \leq -1$ only). Hence the convergence relations given by (4.10) holds for $-1 < x \leq 0$ as well. Consequently we can write

$$\lim_{M\to\infty} \overline{[k/M]} = \lim_{M\to\infty} \overline{[2M - p/M]} = xf_1(x), \qquad -1 < x < \infty. \tag{4.11}$$

REMARK 3. For fixed k $(k = 0, ..., 2M)$ the approximants $[k/M]$ and $\overline{[k/M]}$, while for fixed p $(p = 0, ..., 2M)$ the approximants $[2M - p/M]$ and $\overline{[2M - p/M]}$

converge to the Stieltjes function $xf_1(x)$ for $-1 < x < \infty$, as M goes to infinity, cf. (4.9), (4.10) and (4.11). □

In the next section the properties of the convergence of $[k/M]$, $\overline{[k/M]}$, $[2M-p/M]$, and $\overline{[2M-p/M]}_{2M-p}$ will be investigated. To this end the continued fractions (4.3) and (4.4), the restrictions (2.3) and (4.7), and the convergence relations (4.9) – (4.11) will be used.

5. Two-point Padé bounds on $xf_1(x)$

For simultaneous representation of the sequences $[k/M]$, $[M+r/M]$, $[2M-p/M]$ $\{\overline{[k/M]}, \overline{[M+r/M]}, \overline{[2M-p/M]}\}$ it is convenient to introduce the notation $[I_M/M]$ $\{\overline{[I_M/M]}\}$, where $I_M = k,\ M+r,\ 2M-p$. Now we are prepared to formulate the fundamental theorem establishing $2PAs$ and $\overline{2PAs}$ bounds on $xf_1(x) = \lambda_e(x)/\lambda_1 - 1$, cf. (2.2):

THEOREM 1. *For $I_M = k,\ M+r,\ 2M-p$ $(0 \le I_M \le 2M,\ M \ge |r|)$ the Padé approximants $[I_M/M]$ and $\overline{[I_M/M]}$ (cf. Defs. 1 and 2)) to the power expansions of $xf_1(x)$ at $x=0$ and $x=\infty$ (cf. (2.4) and (2.6)) obey the following inequalities, where $xf_1(x)$ stands for the limit of $[I_M/M]$ and $\overline{[I_M/M]}$, as M tends to infinity:*

(i) *If* $-1 < x < 0$ *then*

$$[I_M/M] - [I_{M+1}/M+1] > 0, \tag{5.1}$$

$$\overline{[I_M/M]} - \overline{[I_{M+1}/M+1]} < 0, \tag{5.2}$$

$$[I_M/M] > xf_1(x) > \overline{[I_M/M]}. \tag{5.3}$$

(ii) *If* $0 < x < \infty$ *then*

$$(-1)^{I_{M+1}}[I_{M+1}/M+1] - (-1)^{I_M}[I_M/M] > 0, \tag{5.4}$$

$$(-1)^{I_{M+1}}\overline{[I_{M+1}/M+1]} - (-1)^{I_M}\overline{[I_M/M]} < 0, \tag{5.5}$$

$$(-1)^{I_M}[I_M/M] < (-1)^{I_M}xf_1(x) < (-1)^{I_M}\overline{[I_M/M]}. \tag{5.6}$$

The inequalities (5.1) – (5.2) *and* (5.4) – (5.5) *have a consequence that the bounds* $[I_M/M]$ $\{\overline{[I_M/M]}\}$ *are the best with respect to the given coefficients p of the power series* (2.4) *and terms k of the power expansion* (2.6), *and that the use of additional input data (higher p and k) improves the bounds on $xf_1(x)$.*

P r o o f. As an example, the inequality (5.2), $I_M = 2M-p$ will be proved only. The remaining inequalities one can prove in a similar manner. Let us start from the continued fractions (4.3)

$$\begin{aligned}\overline{[2M-p/M]} &= \frac{xG_1}{1+xG_2} \; + \ldots + \; \frac{xT_{2M+1}}{1}\,,\\ \overline{[2M+2-p/M+1]} &= \frac{xG_1}{1+xG_2} \; + \ldots + \; \frac{d_{2M+1}}{1} \; + \; \frac{d_{2M+2}}{x} \; + \; \frac{xT_{2M+3}}{1}\,.\end{aligned} \tag{5.7}$$

Of interest is the difference $\delta(x)$ given by (see (5.7))

$$(5.8) \qquad \delta(x) = \frac{d_{2M+1}}{1} + \frac{d_{2M+2}}{x} + \frac{xT_{2M+3}}{1} - \frac{xT_{2M+1}}{1} \\ = x\left(\frac{d_{2M+1}(1+T_{2M+3})}{x(1+T_{2M+3})+d_{2M+2}} - T_{2M+1}\right).$$

On the basis of (4.5) and (4.7) we have

$$(5.9) \qquad \begin{aligned} &\frac{d_{2M+1}(1+T_{2M+3})}{x(1+T_{2M+3})+d_{2M+2}} - T_{2M+1} = 0, &&\text{if} \quad x=-1, \\ &\frac{d_{2M+1}(1+T_{2M+3})}{x(1+T_{2M+3})+d_{2M+2}} - T_{2M+1} < 0, &&\text{if} \quad -1 < x < \infty. \end{aligned}$$

The relations (5.9), the restrictions (4.7) and the recurrence formula for the continued fractions (5.7) lead immediately to the inequality (5.2), $I_M = 2M - p$. The remaining inequalities, namely (5.1), (5.2), $I_M = k$, $M + r/M$, (5.4) and (5.5), can be proved analogously. The relations (5.3) and (5.6) are direct consequence of (4.9), (4.11), (5.1) – (5.2) and (5.4) – (5.5).

Now we are prepared to prove that, with respect to a given number of coefficients of power series (2.4) and (2.6), the $2PAs$ and $\overline{2PAs}$ provide the best estimations for $xf_1(x)$. Assume that $[k_1/M_1]$ $\{[k_2/M_2]\}$ is determined by p_1 $\{p_2\}$ coefficients of (2.4) and k_1 $\{k_2\}$ coefficients of (2.6), where $p_1 + k_1 = 2M_1$, $p_2 + k_2 = 2M_2$, $p_1 \le p_2$ and $k_1 \le k_2$. Of interest is the following scheme of transition of $[k_1/M_1]$ to $[k_2/M_2]$:

$$[k_1/M_1] \to [k_1/M'] = [2M' - p_2/M'] \to [2M' - p_2/M_2] = [k_2/M_2],$$

where $M_1 \le M' \le M_2$. By applying the inequalities (5.1) – (5.3) and (5.4) – (5.6) successively to the above transition scheme, we arrive at

$$(5.10) \qquad |xf_1(x) - [k_1/M_1]| \ge |xf_1(x) - [k_2/M_2]|.$$

Analogously we obtain

$$(5.11) \qquad |xf_1(x) - \overline{[k_1/M_1]}| \ge |xf_1(x) - \overline{[k_2/M_2]}|.$$

From (5.10) – (5.11), it follows that for $p_2 \ge p_1$ and $k_2 \ge k_1$ the estimations $[k_2/M_2]$, $\overline{[k_2/M_2]}$ of $xf_1(x)$ are better than $[k_1/M_1]$, $\overline{[k_1/M_1]}$. □

For a better understanding of Th. 1 it is convenient to arrange Padé approximants $[k/M]$ and $\overline{[k/M]}$ in the following triangular array

$$
\begin{array}{ccccc}
 & & & 0/3 & \dots \\
 & & 0/2 & 1/3 & \dots \\
 & 0/1 & 1/2 & 2/3 & \dots \\
0/0 & 1/1 & 2/2 & 3/3 & \dots \\
 & 2/1 & 3/2 & 4/3 & \dots \\
 & & 4/2 & 5/3 & \dots \\
 & & & 6/3 & \dots
\end{array}
\tag{5.12}
$$

called $2PAs$-table if $k/M = [k/M]$, or $\overline{2PAs}$-table, if $k/M = \overline{[k/M]}$. The sequence M/M is named the main row. Besides M/M one finds the sequences $M+r/M$, k/M and $2M-p/M$ constituting the r-th rows, the diagonals going up and the diagonals going down. Note that the sequences $0/M$ and $1/M$ represent the classical Milton's estimations of $xf_1(x)$, cf. [24], while $0/1$ are the well known Hashin – Shtrikman bounds on $xf_1(x)$, cf. [17]. The remaining bounds appearing in (5.12) are new.

6. General power expansions of $xf_1(x)$

The most general input data for evaluation of the $2PAs$ and $\overline{2PAs}$ to $xf_1(x)$ are given by:

$$
\begin{aligned}
xf_1(x) &= \sum_{n=1}^{\infty} c_n^{(1)} x^n, \\
xf_1(x) &= \sum_{n=0}^{\infty} C_{n\nu}^{(1)} s_\nu^n, \qquad s_\nu = 1/(x-\nu).
\end{aligned}
\tag{6.1}
$$

Here ν is an arbitrary, non-negative number. Since $(6.1)_1$ coincides with (2.4), of interest is the expansion $(6.1)_2$ only. From (2.6) and $(6.1)_2$ we have

$$
\begin{aligned}
xf_1(x) &= \sum_{n=0}^{\infty} C_n^{(1)} s^n = \sum_{n=0}^{\infty} C_{n\nu}^{(1)} s_\nu^n, \\
s &= \frac{1}{x}, \qquad s_\nu = \frac{1}{x-\nu}, \qquad s_\nu = \frac{s}{1-s\nu}.
\end{aligned}
\tag{6.2}
$$

Equality (6.2) provides the following recurrence formulae interrelating the coefficients $C_n^{(1)}$ and $C_{k\nu}^{(1)}$:

$$
C_0^{(1)} = C_{0\nu}^{(1)}, \qquad C_1^{(1)} = C_{1\nu}^{(1)},
\tag{6.3}
$$

$$C_n^{(1)} = \sum_{k=1}^{n} \nu^{n-k} A_n^k C_{k\nu}^{(1)}, \qquad n = 2, 3, ..., \tag{6.4}$$

where

$$A_n^k = \begin{cases} 1, & \text{if} \quad k = 1, \\ A_{n-1}^{k-1} + A_{n-1}^{k}, & \text{if} \quad k = 2, 3, ..., n-1, \\ 1, & \text{if} \quad k = n. \end{cases} \tag{6.5}$$

From (6.3) – (6.5) it follows:

REMARK 4. Any power expansions of $xf_1(x)$ at $x = 0$ and $x = \infty$ given by (6.1), ($\nu > 0$) can always be reduced to the standard ones (6.1), ($\nu = 0$), cf. (2.4) and (2.6). It means that $2PAs$ and $\overline{2PAs}$ to power series (6.1), ($\nu \geq 0$) do not depend on ν.

7. Physical example

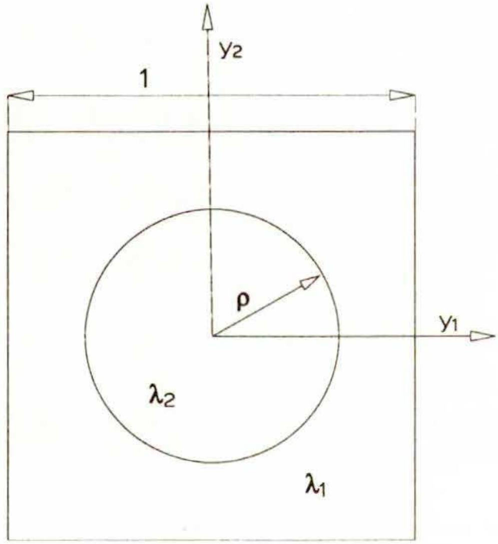

FIG. 1. Unit cell for a square array of cylinders.

In this section we evaluate low order Padé bounds $[k/M]$ and $\overline{[k/M]}$ on the effective conductivity $\lambda_e(x)/\lambda_1$ of a composite material consisting of equally-sized cylinders embedded in an infinite matrix, cf. Fig. 1. To this end we set: $\phi = \pi\varrho^2$ – volume fraction of inclusions, ϱ – the radius of cylinders, λ_1, λ_2 conductivity of the matrix and inclusions, $x = (\lambda_2/\lambda_1) - 1$ – normalized physical properties of the composite components. Two coefficients of the expansion of $\lambda_e(x)/\lambda_1$ at $x = 0$ are reported in [4],

$$x f_1(x) = \frac{\lambda_e(x)}{\lambda_1} - 1 = c_1^{(1)} x + c_2^{(1)} x^2 + O(x^3), \tag{7.1}$$
$$c_1^{(1)} = \phi = \pi \varrho^2, \qquad c_2^{(1)} = \xi = -0.5\phi(1-\phi),$$

while at $x = \infty$ in [22]

$$x f_1(x) = \frac{\lambda_e(x)}{\lambda_1} - 1 = C_0^{(1)} + C_1^{(1)} \frac{1}{x} + O\left(\frac{1}{x}\right)^2,$$
$$C_0^{(1)} = A = [\pi(w-1) - 1], \tag{7.2}$$
$$C_1^{(1)} = B = -2\pi w(w-1)\ln(w), \qquad w = \sqrt{\pi/(\pi - 4\phi)}.$$

Low order $2PAs$ and $\overline{2PAs}$ bounds corresponding to (7.1) and (7.2) are given by:

$$[0/0] = 1, \qquad \overline{[0/0]} = x,$$
$$[0/1] = \frac{\phi x}{1 + 0.5(1-\phi)x}, \qquad \overline{[0/1]} = \frac{\phi x + 0.5\phi x^2}{1 + x - 0.5\phi x},$$
$$[1/1] = \frac{\phi x}{1 + (\phi/A)x}, \qquad \overline{[1/1]} = \frac{\phi x}{1 + (1-\phi)x},$$
$$[2/1] = -\frac{(A^2/B)x}{1 - (A/B)x}, \qquad \overline{[2/1]} = \frac{Ax}{1 + A + x}, \tag{7.3}$$
$$[2/2] = \frac{G_1 x + G_1 G_4 x^2}{1 + (G_2 + G_3 + G_4)x + G_2 G_4 x^2},$$
$$\overline{[2/2]} = \frac{G_1 x + G_1(G_4 + V_5)x^2}{1 + (G_2 + G_3 + G_4 + V_5)x + G_2(G_4 + V_5)x^2},$$

where

$$G_1 = \phi, \qquad G_2 = \frac{\phi}{A}, \qquad G_3 = -\frac{\phi}{A} - \frac{\xi}{\phi}, \tag{7.4}$$

$$G_4 = \frac{\phi^2 + A\xi}{A^2 + \phi B}\,\frac{A}{\phi}, \qquad V_5 = 1 - G_4 - \frac{G_3}{1 - G_1 - G_2}. \tag{7.5}$$

For $\phi = 0.7853$ $2PAs$ and $\overline{2PAs}$ given by (7.3) are depicted in Figs. 2 and 3. It follows that for $x > 0$ the upper Padé estimation $1 + \overline{[2/2]}$ of $\lambda_e(x)/\lambda_1$ provides the significant improvement over the upper Hashin - Shtrikman bound $1 + \overline{[0/1]}$. Moreover, for $x \to \infty$ the Padé bound $1 + \overline{[2/2]}$ takes finite values, while the Hashin - Shtrikman bound $1 + \overline{[0/1]}$ goes to infinity. We have to add that in our previous papers the only $2PAs$ bounds on $x f_1(x)$ have been investigated [28, 29]. The two-point Padé bounds of the type $\overline{2PAs}$, used in this paper, are new.

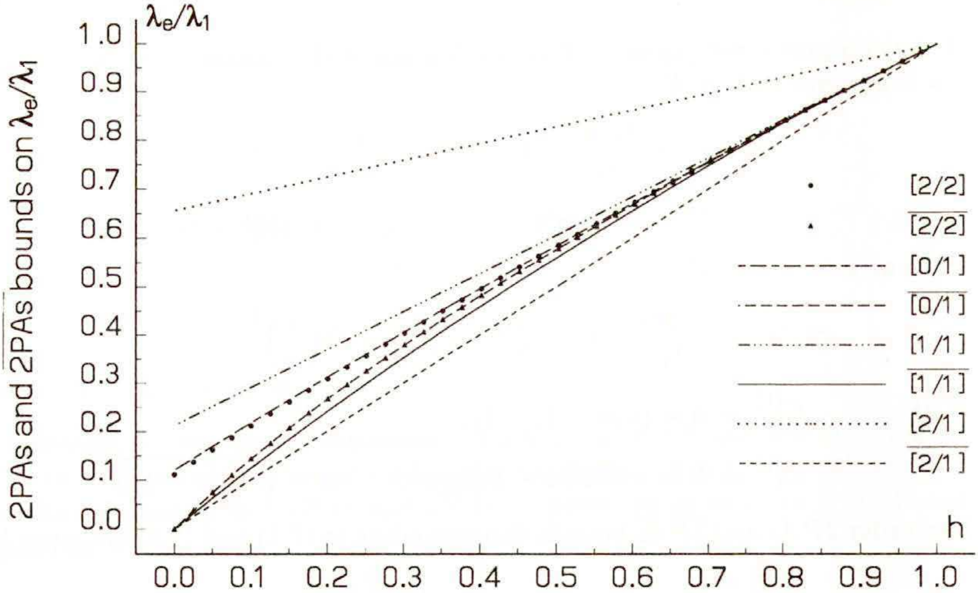

FIG. 2. Low order $2PAs$ and $\overline{2PAs}$ bounds on the effective conductivity $\lambda_e(x)/\lambda_1$ of a square array of densely spaced cylinders – a comparison with Hashin–Sthrikman estimations $1 + [0/1]$ and $1 + \overline{[0/1]}$; $\phi = 0.7853$, $h < 1$.

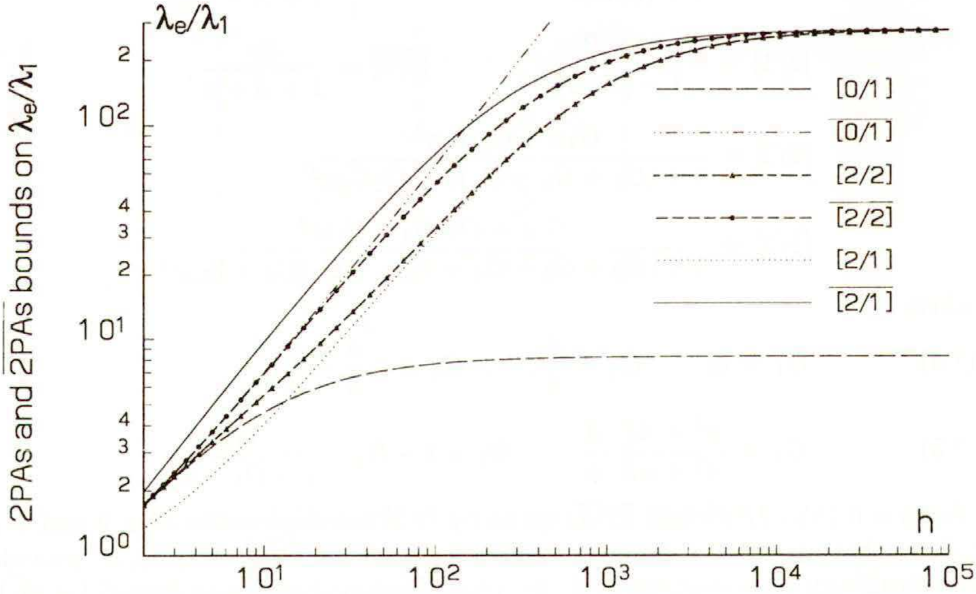

FIG. 3. Low order $2PAs$ and $\overline{2PAs}$ bounds on the effective conductivity $\lambda_e(x)/\lambda_1$ of a square array of densely spaced cylinders – a comparison with Hashin–Sthrikman estimations $1 + [0/1]$ and $1 + \overline{[0/1]}$; $\phi = 0.7853$, $h > 1$.

8. Conclusions

The main result of this paper, formulated as Th. 1 establishes, in terms of two-point Padé approximants $2PAs$ and $\overline{2PAs}$, the new bounds on the real-valued moduli $\lambda_e(x)/\lambda_1$ of two-phase media. The bounds achieved are the best possible with respect to the given number of coefficients of the power expansions of $\lambda_e(x)/\lambda_1$ at $x = 0$ and $x = \infty$. Moreover, for $x > 0$ they provide a significant improvement over the corresponding ones reported in the literature, cf. [24].

If the orientation of the principal axis of a composite does not depend on the properties of components, $2PAs$ and $\overline{2PAs}$ can be used for estimation of the principal values of a second-rank tensors, i.e. for bounding the anisotropic transport coefficients.

For a power expansion of $\lambda_e(x)/\lambda_1$ available at $x = 0$ only, $2PAs$ and $\overline{2PAs}$ to $\lambda_e(x)/\lambda_1$ reduce to the classical bounds on $\lambda_e(x)/\lambda_1$ originally derived by MILTON in [24].

The $2PAs$ and $\overline{2PAs}$ bounds on $\lambda_e(x)/\lambda_1$ can be improved by incorporating the additional information about the composite such as the Keller identity for two-dimensional system or the Schulgasser inequality for three-dimensional ones, cf. [7] and [9]. The Keller's and Schulgasser's restrictions and their influence on the Padé bounds on $\lambda_e(x)/\lambda_1$ will be investigated in a separate paper.

Acknowledgment

The authors were supported by the State Committee for Scientific Research through the Grant No. 7 T07A 016 12 and through the fund for Polish-Ukrainian cooperation No. 4222/DZ/95.

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Received November 27, 1996.