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Bounds on the effective transport coefficients of two-phase media from discrete theoretical and experimental data

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By applying Padé approximants and continued fractions technique developed in [1, 2, 3, 24] we investigate a composite material of the effective modulus $\lambda_e(h)$ consisting of two components of real moduli λ_1 and λ_2, respectively, where $h = \lambda_2/\lambda_1$. By starting from K power expansions of $\lambda_e(h)$ at fixed points $h = h_1, h_2, \ldots, h_K$ the infinite set of the general inequalities specifying explicitly the upper and lower bounds on $\lambda_e(h)/\lambda_1$ are derived. Our estimations generalize the previous bounds reported in [13, 17, 22]. The inequalities achieved are applied for the evaluation of the upper and lower bounds on $\lambda_e(h)/\lambda_1$ from the given experimental measurements.

1. Introduction

In view of the difficulty in calculating the effective parameters $\lambda_e(h), h = \lambda_2/\lambda_1$(such as dielectric constant, magnetic permeability, thermal or electrical conductivity) for two-phase medium consisting of components of moduli of λ_1 and λ_2, there has been much interest in obtaining bounds on these parameters. Wiener [24] derived optimal bounds on $\lambda_e(h)$ with fixed volume fractions and real components parameters. These bounds are known as the arithmetic and harmonic mean bounds. For isotropic materials, Hashin and Shtrikman [13] improved Wiener's bounds using variational principles. Bergman [4, 5, 6,] introduced a method for obtaining bounds on $\lambda_e(h)$ which does not rely on variational principles. Instead it makes use of the properties of the effective parameters as analytic functions of the components moduli. The method of Bergman was studied in detail and applied to several problems by Milton [16, 17]. A rigorous mathematical formulation of Bergman's approach was given by Golden and Papanicolaou [11]. Recently several interesting continued fraction techniques for evaluation of the bounds on $\lambda_e(h)$ have been presented by Bergman [7] for three- and Clark and Milton [8], — for two-dimensional systems. Both Milton [17] and Bergman [7] have incorporated into the bounds a power expansion of $\lambda_e(h)$ at $h = 1$ and the discrete values $\lambda_e(h_1), \lambda_e(h_2), \ldots, \lambda_e(h_K)$ only.

The purpose of this paper is to derive, from the power expansions of $\lambda_e(h)$ at K points $h = h_1, h_2, \ldots, h_K$, an infinite set of general inequalities expressing the best bounds on $\lambda_e(h)$. Those inequalities generalize Milton's and Bergman's results [7, 17]. As an application, on the basis of the available experimental measurements, the bounds on $\lambda_e(h)$ for a hexagonal array of cylinders are evaluated.

2. Preliminaries: notations and basic definitions

Let us denote by Λ_e the effective conductivity of a composite consisting of two isotropic components of conductivities λ_1, λ_2 with volume fractions φ_2 and $\varphi_1 = 1-\varphi_2$, respectively. The bulk moduli Λ_e are defined from the linear relationship between the volume-averaged temperature gradient $< \nabla T >$ and the volume-averaged heat flux $< J >$:

$$< J >= \Lambda_e < \nabla T > . \tag{1}$$

The average value $< . >$ is calculated over a representative volume or a basic cell. In general Λ_e is a second-order symmetric tensor, even when λ_1 and λ_2 are both scalars, and depends on the microstructure of composite. Focusing upon one of the principal values of Λ_e, say λ_e, we can write the following K Stieltjes integrals

$$F_j(h-h_j) = 1 + (h-1)\int_0^{1/h_j} \frac{d\gamma_j(u)}{1+(h-h_j)u}, \quad h = \frac{\lambda_2}{\lambda_1} \in (0,\infty), \quad j = 1,2,\ldots,K, \tag{2}$$

representing the effective conductivity $\lambda_e(h)/\lambda_1$, cf. [1, Lemma 17.1] and [11, 12],

$$\frac{\lambda_e(h)}{\lambda_1} = F(h) = F_j(h-h_j), \quad (j = 1,2,\ldots,K). \tag{3}$$

For further development we assume that

$$h_0 < h_1 < h_2 < \ldots < h_{K-1} < h_K < h_{K+1}, \quad h_0 = 0, \quad h_{K+1} = \infty . \tag{4}$$

The spectra $\gamma_j(u)$ $(j = 1,2,\ldots,k)$ are real, bounded and non-decreasing functions determined for $0 \le u < \infty$. The power expansions of $F_j(h-h_j)$ at $h = h_j$ $(j = 1,2,\ldots,K)$ take the following form

$$F_j(h-h_j) = \sum_{n=0}^{\infty} F_{jn}(h-h_j)^n = 1 + (h-1)\sum_{n=0}^{\infty} f_{jn}(h-h_j)^n, \quad j = 1,2,\ldots,K, \tag{5}$$

where coefficients F_{jn} and f_{jn} are interrelated by:

(i) If $h_j - 1 \neq 0$ $(j = 1,2,\ldots,K)$, then

$$f_{j(-1)} = 1, \quad f_{jn} = \frac{F_{jn} - f_{j(n-1)}}{h_j - 1}, \quad n = 0,1,\ldots \tag{6}$$

(ii) If $h_j - 1 = 0$ $(j = 1,2,\ldots,K)$, then

$$f_{j(-1)} = 1, \quad f_{j(n-1)} = F_{jn}, \quad n = 0,1,\ldots . \tag{7}$$

Here f_{jn} are moments of the spectra $d\gamma_j$, cf. (2) and (5)

$$f_{jn} = (-1)^n \int_0^{1/h_j} u^n d\gamma_j(u), \quad j = 1,2,\ldots,K; \quad n = 0,1,2,\ldots . \tag{8}$$

Let us consider the power expansions $f_j(h-h_j)$ $(j = 1,2,\ldots,K)$ of the Stieltjes function $f(h)$ given by (5)

$$f(h) = f_j(h-h_j) = \frac{F_j(h-h_j)-1}{h-1} = \sum_{n=0}^{\infty} f_{jn}(h-h_j)^n, \quad h \in (0,\infty). \tag{9}$$

Subdiagonal and diagonal K-point Padé approximants $\Lambda^{N_1,N_2,\ldots,N_K}_{h_1,h_2,\ldots,h_K}(h)$ to Stieltjes function $f(h)$ represented by (9), constructed from $N_1, N_2, \ldots, N_K$ coefficients of the Stieltjes series $f_1(h-h_1), f_2(h-h_2), \ldots, f_K(h-h_K)$ respectively, are given by

$$\Lambda^{N_1,N_2,\ldots,N_K}_{h_1,h_2,\ldots,h_K}(h) = \frac{a_0^I + a_1^I h + \cdots + a_M^I h^M}{1 + b_1^I h + \cdots + b_{M+I}^I h^{M+I}}, \tag{10}$$

where

$$\begin{aligned} M &= \frac{(N-1)}{2} \quad \text{and} \quad I = 0, \quad \text{if } N = \sum_{j=1}^{K} N_j \text{ is odd,} \\ M &= \frac{(N-2)}{2} \quad \text{and} \quad I = 1, \quad \text{if } N = \sum_{j=1}^{K} N_j \text{ is even.} \end{aligned} \tag{11}$$

Let us consider K power expansions of $\Lambda^{N_1,N_2,\ldots,N_K}_{h_1,h_2,\ldots,h_K}(h)$ at $h = h_j$ $(j = 1, 2, \ldots, K)$

$$\Lambda^{N_1,N_2,\ldots,N_K}_{h_1,h_2,\ldots,h_K}(h) = \sum_{n=0}^{\infty} G^I_{jn}(h-h_j)^n, \quad I = 0,1, \quad j = 1,2,\ldots,K. \tag{12}$$

The rational function $\Lambda^{N_1,N_2,\ldots,N_K}_{h_1,h_2,\ldots,h_K}(h)$ is the K-point Padé approximant to K power series (9), provided that, cf. [1, Chap. 17],

$$G^I_{jn,I} = f_{jn}, \quad n = 0,1,\ldots,N_j - 1, \quad j = 1,2,\ldots,K, \quad I = 0,1. \tag{13}$$

On the basis of [1, Chap. 17B] K-point Padé approximants defined by (10)–(13) have the following continued fraction representation,

$$\begin{aligned} &\Lambda^{N_1,N_2,\ldots,N_K}_{h_1,h_2,\ldots,h_K}(h) = \\ &\frac{g_{1,1}(h-h_1)}{1} \;+\; \frac{g_{1,2}(h-h_1)}{1} \;+\cdots+\; \frac{g_{1,N_1}(h-h_1)}{1} \;+ \\ &\frac{g_{2,1}(h-h_1)}{1} \;+\; \frac{g_{2,2}(h-h_2)}{1} \;+\cdots+\; \frac{g_{2,N_2}(h-h_2)}{1} \;+ \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ &\frac{g_{K,1}(h-h_{K-1})}{1} \;+\; \frac{g_{K,2}(h-h_K)}{1} \;+\cdots+\; \frac{g_{K,N_K}(h-h_K)}{1}. \end{aligned} \tag{14}$$

The above specific notation for Padé approximants is clarified in detail in [1–3]. Parameters $g_{n,j}$ appearing in (14) are uniquely determined by $N_1, N_2, \ldots, N_K$ coefficients of the Stieltjes series (9) $(j = 1, 2, \ldots, K)$. Moreover the parameters $g_{n,j}$ are positive, cf. [1, Chap.17],

$$g_{n,j} > 0, \quad n = 1,2,\ldots,N_j; \quad j = 1,2,\ldots,K. \tag{15}$$

3. Continued fractions bounds on $\lambda_e(h)/\lambda_1$

Now we are prepared to introduce a continued fraction operator $S^p_n(\,.\,)$

$$S^p_n(\,.\,) = \frac{g_{n,1}(h-h_n)}{1} \;+\; \frac{g_{n,2}(h-h_n)}{1} \;+\cdots+\; \frac{g_{n,p}(h-h_n)}{1+(\,.\,)(h-h_n)}. \tag{16}$$

From (14) and (16), it follows

$$S_1^{N_1} S_2^{N_2} \ldots S_K^{N_K}(0) = \Lambda^{N_1,N_2,\ldots,N_K}_{h_1,h_2,\ldots,h_K}(h). \tag{17}$$

Of an additional interest is the continued fraction $\overline{\Lambda}^{N_1,N_2,\dots,N_K}_{h_1,h_2,\dots,h_K}(h)$ defined by

$$S_1^{N_1}S_2^{N_2}\dots S_K^{N_K}(V_{K,N_K+1}) = \overline{\Lambda}^{N_1,N_2,\dots,N_K}_{h_1,h_2,\dots,h_K}(h) = \frac{g_{1,1}(h-h_1)}{1} \underset{+}{} \frac{g_{1,2}(h-h_1)}{1} \underset{+}{} \dots \underset{+}{} \frac{g_{1,N_1}(h-h_1)}{1} \underset{+}{} \frac{g_{2,1}(h-h_1)}{1} \underset{+}{} \frac{g_{2,2}(h-h_2)}{1} \underset{+}{} \dots \underset{+}{} \frac{g_{2,N_2}(h-h_2)}{1} \underset{+}{} \dots \frac{g_{K,1}(h-h_{K-1})}{1} \underset{+}{} \frac{g_{K,2}(h-h_K)}{1} \underset{+}{} \dots \underset{+}{} \frac{g_{K,N_K}(h-h_K)}{1+V_{K,N_K+1}(h-h_K)}, \tag{18}$$

where parameter V_{K,N_K} satisfies the relations

$$\left|S_1^{N_1}S_2^{N_2}\dots S_K^{N_K}(V_{K,N_K+1})\right|_{h=0} = -1, \quad V_{K,N_K+1} > 0. \tag{19}$$

It has been shown in [1, Chap. 17] that the Stieltjes function $f(h)$ given by (9) takes values within the following limits

$$S_1^{N_1}S_2^{N_2}\dots S_K^{N_K}(0) \quad \text{and} \quad S_1^{N_1}S_2^{N_2}\dots S_K^{N_K}(V_{K,N_K+1}), \quad 0 < h < \infty. \tag{20}$$

For a fixed h and known h_j, N_j $(j = 1, 2, \dots, K)$, it is of interest, which formulae given by $(20)_1$ and $(20)_2$ represent the upper and lower estimations for $f(h)$. To answer this question, let us introduce new notations for the Stieltjes series $f_j(h-h_j)$, cf. (9),

$$f_j(h-h_j) = f_j^{(1,1)}(h-h_j). \tag{21}$$

Consider now the function $f_K^{(K,N_K+1)}(h-h_k)$ defined by

$$f_1^{(1,1)}(h-h_1) = S_1^{N_1}S_2^{N_2}\dots S_K^{N_K}\left(f_K^{(K,N_K+1)}(h-h_k)\right). \tag{22}$$

From relations (15), (19) and the analytical property $\lambda_e(0)/\lambda_1 \geq 0$, it follows that

$$0 \leq f_K^{(K,N_K+1)}(h-h_k) \leq V_{K,N_K+1}. \tag{23}$$

The inequality (23) allows us to formulate

Lemma 1. *The estimations $(20)_1$ and $(20)_2$ of the function $f(y)$ (9) obey at fixed $h \in (h_r, h_{r+1})$, $0 \leq r \leq K$ the following inequalities:*

$$\begin{aligned} (-1)^R f_1(h) &\leq (-1)^R S_1^{N_1}S_2^{N_2}\dots S_K^{N_K}(V_{K,N_K+1}), \\ (-1)^R f_1(h) &\geq (-1)^R S_1^{N_1}S_2^{N_2}\dots S_K^{N_K}(0), \end{aligned} \tag{24}$$

where

$$R = \sum_{j=0}^{r} N_j, \; N_0 = 0, \; h_0 = 0, \; h_{K+1} = \infty. \tag{25}$$

Proof: The relations (24)–(25) are a direct consequence of the relation (15), the recurrence formulae for the continued fractions (17)–(18) and the inequality (23).

4. Inequalities for effective moduli $\lambda_e(h)/\lambda_1$

Now we are prepared to formulate the general inequalities for the effective transport coefficients $\lambda_e(h)/\lambda_1$ of two-phase media.

Theorem 1. *The effective moduli $\lambda_e(h)/\lambda_1$ of two-phase media satisfy at fixed $h \in (h_r, h_{r+1})$, $0 \leq r \leq K$ the following general inequalities:*

(i) *If $h_r < h < h_{r+1}$ and $0 < h < 1$, then*

$$(-1)^R \frac{\lambda_e(h)}{\lambda_1} \geq (-1)^R \left[1 + (h-1) S_1^{N_1} S_2^{N_2} \dots S_K^{N_K}(V_{K,N_K+1})\right],$$
$$(-1)^R \frac{\lambda_e(h)}{\lambda_1} \leq (-1)^R \left[1 + (h-1) S_1^{N_1} S_2^{N_2} \dots S_K^{N_K}(0)\right]. \tag{26}$$

(ii) *If $h_r < h < h_{r+1}$ and $1 < h < \infty$, then*

$$(-1)^R \frac{\lambda_e(h)}{\lambda_1} \leq (-1)^R \left[1 + (h-1) S_1^{N_1} S_2^{N_2} \dots S_K^{N_K}(V_{K,N_K+1})\right],$$
$$(-1)^R \frac{\lambda_e(h)}{\lambda_1} \geq (-1)^R \left[1 + (h-1) S_1^{N_1} S_2^{N_2} \dots S_K^{N_K}(0)\right], \tag{27}$$

where as previously, R and h_{K+1} are given by (25).

Proof: From Lemma 1 and the definitions (3) and (9), follow directly the inequalities (26)–(27).

With respect to the available parameters h, N_j and h_j $(j = 1, 2, \dots, K)$, the general inequalities (26)–(27) identify explicitly the estimations

$$1 + (h-1) S_1^{N_1} S_2^{N_2} \dots S_K^{N_K}(V_{K,N_K+1}) \quad \text{and} \quad 1 + (h-1) S_1^{N_1} S_2^{N_2} \dots S_K^{N_K}(0) \tag{28}$$

as the upper and lower bounds on $\lambda_e(h)/\lambda_1$, respectively. The derived formulae (26)–(27) are the main theoretical result of the present paper.

5. Particular cases of the general inequalities

Now we are in position to investigate the particular cases of the general inequalities (26)–(27). At the input data given by

$$N_j = 1, \quad \text{if} \quad h_j \neq 1, (j = 1, \dots, n-1),$$
$$N_n \geq 1 \quad \text{if} \quad h_n = 1, \tag{29}$$
$$N_j = 1, \quad \text{if} \quad h_j \neq 1, (j = n+1, \dots, K)$$

the relations (26)–(27) take the form:

(i) If $0 < h < 1$ and $h_r < h < h_{r+1}$, then

$$(-1)^R \frac{\lambda_e(h)}{\lambda_1} \geq (-1)^R \left[1 + (h-1) S_1^1 \dots S_n^{N_n} \dots S_K^1(V_{K,N_K+1})\right],$$
$$(-1)^R \frac{\lambda_e(h)}{\lambda_1} \leq (-1)^R \left[1 + (h-1) S_1^1 \dots S_n^{N_n} \dots S_K^1(0)\right], \tag{30}$$

(ii) If $1 < h$ and $h_r < h < h_{r+1}$, then

$$(-1)^R \frac{\lambda_e(h)}{\lambda_1} \leq (-1)^R \left[1 + (h-1) S_1^1 \dots S_n^{N_n} \dots S_K^1(V_{K,N_K+1})\right],$$
$$(-1)^R \frac{\lambda_e(h)}{\lambda_1} \geq (-1)^R \left[1 + (h-1) S_1^1 \dots S_n^{N_n} \dots S_K^1(0)\right], \tag{31}$$

By inserting the input parameters

$$N_1 \geq 1 \quad \text{for} \quad h_1 = 1 \tag{32}$$

into (26)–(27), one obtains

$$1+(h-1)S_1^{N_1}(0) \;\geq\; \frac{\lambda_e(h)}{\lambda_1} \;\geq 1+(h-1)S_1^{N_1}(V_{K,N_K+1}), \quad 0<h<1, \tag{33}$$

$$\begin{aligned}(-1)^{N_1}\,\frac{\lambda_e(h)}{\lambda_1} \;&\leq\; (-1)^{N_1}\left[1+(h-1)S_1^{N_1}(V_{K,N_K+1}\right],\\ & \qquad\qquad\qquad\qquad\qquad 1<h,\\ (-1)^{N_1}\,\frac{\lambda_e(h)}{\lambda_1} \;&\geq\; (-1)^{N_1}\left[1+(h-1)S_1^{N_1}(0)\right].\end{aligned} \tag{34}$$

The right-hand sides of (30)–(31) and (33)–(34) coincide with the well known estimations of $\lambda_e(h)/\lambda_1$originally derived by Milton in [17]. For

$$N_1 = 1 \quad \text{for} \quad h_1 = 1 \qquad \text{and} \qquad N_1 = 2 \quad \text{for} \quad h_1 = 1, \tag{35}$$

the inequalities (26)–(27) reduce to the Wiener [24]

$$1+(h-1)S_1^1(0) \;\geq\; \frac{\lambda_e(h)}{\lambda_1} \;\geq\; 1+(h-1)S_1^1(V_{K,N_K+1}), \quad 0 \leq h < \infty \tag{36}$$

and Hashin-Shtrikman bounds [13]

$$\begin{aligned}1+(h-1)S_1^2(0) \geq \frac{\lambda_e(h)}{\lambda_1} \geq 1+(h-1)S_1^2(V_{K,N_K+1}), \quad 0<h<1,\\ 1+(h-1)S_1^2(0) \leq \frac{\lambda_e(h)}{\lambda_1} \leq 1+(h-1)S_1^2(V_{K,N_K+1}), \quad 1<h<\infty.\end{aligned} \tag{37}$$

The general inequalities (26)–(27) and the particular ones (30)–(31), (33)–(34) specify, with respect to the available h, h_j and N_j, the upper and lower estimations for $\lambda_e(h)/\lambda_1$. Such a general specification of the bounds on $\lambda_e(h)/\lambda_1$ has not been available earlier.

6. Recurrence formulae for evaluation of bounds on $\lambda_e(h)$

Let us consider the Stieltjes series given by, cf. (9) and (22),

$$f_m^{(1,1)}(h-h_m) = \sum_{n=0}^{\infty} f_{mn}^{(1,1)}(h-h_m)^n, \tag{38}$$

and a class of Stieltjes expansions

$$f_m^{(i,j)}(h-h_m) = \sum_{n=0}^{\infty} f_{mn}^{(i,j)}(h-h_m)^n \tag{39}$$

defined by:

(i) For $i=1,\; j=1,2,\ldots,N_1$ and $m=1,2,\ldots,K$

$$\begin{aligned}f_m^{(1,j)}(h-h_m) &= \frac{f_1^{(1,j)}(0)}{1+(h-h_1)f_m^{(1,j+1)}(h-h_m)},\\ f_m^{(1,N_1+1)}(h-h_m) &= f_m^{(2,1)}(h-h_m), \quad m=2,3,\ldots,\text{K}.\end{aligned} \tag{40}$$

(ii) For $i = 2,\ j = 1, 2, \ldots, N_2$ and $m = 2, 3 \ldots, K$

$$f_m^{(2,j)}(h - h_m) = \frac{f_2^{(2,j)}(0)}{1 + (h - h_2) f_m^{(2,j+1)}(h - h_m)},$$

....

(iii) For $i = K,\ j = 1, 2, \ldots, N_K$ and $m = K$

$$f_m^{(K,j)}(h - h_m) = \frac{f_K^{(K,j)}(0)}{1 + (h - h_K) f_m^{(K,j+1)}(h - h_m)},$$

where K Stieltjes series (38) are the input data for (40). It is obvious that linear fractional transformations (40) applied to the K series given by (38) lead to a continued fraction (14). Let us start from relations $(40)_1$. By substituting the right-hand sides of (39) into $(40)_1$, for $i = 1$, fixed m ($m = 1, 2, \ldots, K$) and $j = 1, 2, \ldots, N_m$, we obtain the following recurrence formulae:

$$\begin{aligned}
&c_{m0}^{(1,j+1)} = \frac{f_{10}^{(1,j)}}{f_{m0}^{(1,j)}}, \qquad c_{mn}^{(1,j+1)} = -\frac{1}{f_{m0}^{(1,j)}} \sum_{j=0}^{n} c_{mn}^{(1,j+1)} f_{m(n-j)}^{(1,j)}, \\
&f_{m0}^{(1,j+1)} = c_{m0}^{(1,j+1)} - 1, \qquad f_{mn}^{(1,j+1)} = c_{mn}^{(1,j+1)} - f_{m(n-1)}^{(1,j+1)}, \qquad \text{if } m = 1 \\
&f_{m0}^{(1,j+1)} = \frac{c_{m0}^{(1,j+1)} - 1}{h_m - h_1}, \qquad f_{mn}^{(1,j+1)} = \frac{c_{mn}^{(1,j+1)} - f_{m(n-1)}^{(1,j+1)}}{h_m - h_1} \qquad \text{if } m > 1
\end{aligned} \tag{41}$$

for evaluation of parameters $g_{1,j} = f_{10}^{(1,j)}$ $(j = 1, 2, \ldots, N_1)$ of the continued fraction (14) and the coefficients $f_{mn}^{(2,1)}$ of a Stieltjes series $f_m^{(2,1)}(h - h_m)$ $(m = 2, 3, \ldots, K)$

$$f_m^{(2,1)}(h - h_m) = \sum_{n=0}^{\infty} f_{mn}^{(1,N_1+1)} (h - h_m)^n = \sum_{n=0}^{\infty} f_{mn}^{(2,1)} (h - h_m)^n. \tag{42}$$

According to $(40)_2$ the series (42) is a starting point for evaluation of the parameters $g_{2,j}$ $(j = 1, 2, \ldots, N_2)$ of continued fraction (14) and coefficients $f_{mn}^{(3,1)}$ of the Stieltjes series $f_m^{(3,1)}(h - h_m)$, where $m = 3, 4, \ldots, K$

$$f_m^{(3,1)}(h - h_m) = \sum_{n=0}^{\infty} f_{mn}^{(2,N_2+1)} (h - h_m)^n = \sum_{n=0}^{\infty} f_{mn}^{(3,1)} (h - h_m)^n. \tag{43}$$

After K steps we arrive at parameters $g_{n,j}$ $(n = 1, 2, \ldots, K;\ j = 1, 2, \ldots, N_j;\ j = 1, 2, \ldots, K)$ defining the continued fraction (14). It is worth noting that the recurrence relations (40) lead to K-point Padé approximants consisting in a special way of K one-point Padé ones, cf. [1, Chap. 17]. Consequently of interest are the relations given by (41) only.

7. SCHEME OF NUMERICAL EVALUATION OF $G_{M,J}$

Basic recurrence relations for computing the parameters $g_{m,j}$ of the continued fraction (14) from the truncated series (38) are given by

$$\left\{ \begin{array}{l} j = 0, 1, 2, \ldots, N_p - 1, \quad g_{p,j+1} = a_0, \\ \left\{ \begin{array}{l} n = 1, 2, \ldots, N_p - 1 - j, \\ a_{-1}^{(j+2)} = 1, \quad a_n^{(j+2)} = -\dfrac{1}{a_0^{(j+1)}} \left(\displaystyle\sum_{s=-1}^{n-1} a_s^{(j+2)} a_{n-s}^{(j+1)} \right), \end{array} \right. \end{array} \right. \tag{44}$$

and

$$\begin{cases} j=1,2,\ldots,N_m-1, \quad c_0^{(j+1)} = \dfrac{g_{p,j}}{a_0^{(j)}}, \\ \begin{cases} n=1,2,\ldots,N_m-1, \\ c_n^{(j+1)} = -\dfrac{1}{a_0^{(j)}}\displaystyle\sum_{s=0}^{n} c_s^{(j+1)} a_{n-s}^{(j)}, \end{cases} \\ \begin{cases} n=1,2,\ldots,N_m-1, \quad a_0^{(j+1)} = \dfrac{c_0^{(j+1)}-1}{h_m-h_p}, \\ a_n^{(j+1)} = \dfrac{c_n^{(j+1)}-a_{n-1}^{(j+1)}}{h_m-h_p}. \end{cases} \end{cases} \tag{45}$$

Formulae (44) and (45) are a straightforward representation of the recurrence procedure (40). The evaluation of coefficients $g_{p,j}$ of a continued fraction (14) via (44) and (45) goes as follows. First we substitute $a_s^{(1)} = f_{1s}^{(1,1)}$ $(s=1,2,\ldots,N_1)$ into (44) for computing $g_{1,s}$ $(s=1,2,\ldots,N_1)$, next $a_s^{(1)} = f_{ms}^{(1,1)}$ into (45) for getting $f_{ms}^{(2,1)} = a_s^{(N_m+1)}$ $(m=2,3,\ldots,K;\ s=1,2,\ldots,N_m)$. New input data $a_s^{(1)} = f_{2s}^{(2,1)}$ lead via (44) and (45) to the set of parameters $g_{2,s}$ $(s=1,2,\ldots,N_2)$ and set of coefficients $f_{ms}^{(3,1)} = a_s^{(N_m+1)}$ $(m=3,4,\ldots,K;\ s=1,2,\ldots,N_m)$, respectively. By repeating successively the evaluation procedure described above we arrive at $g_{3,s}$ $(s=1,2,\ldots,N_3)$, $g_{4,s}$ $(s=1,2,\ldots,N_4)$, and finally at $g_{K,s}(s=1,2,\ldots,N_K)$. Now we are prepared to compute the coefficient V_{K,N_K} satisfying (19). After some rearrangements of (19) we obtain

$$\begin{cases} m=1,2,\ldots,K,N_m, \\ \begin{cases} j=1,2,\ldots,N_m, \\ V_{m,j+1} = \dfrac{V_{m,j}-g_{m,j}}{V_{m,j}h_m}, \end{cases} \end{cases} \tag{46}$$

where coefficients $g_{m,j}$ and N_m are known, while $V_{1,1}=1$. To complete relations indispensable for evaluation of the bounds on $\lambda_e(h)/\lambda_1$, we demonstrate the last recurrence formulae

$$\begin{cases} m=K,K-1,\ldots,1, \\ \begin{cases} j=0,1,\ldots,N_m-1, \\ Q^{(m,N_m-j)}(h) = \dfrac{g_{m,j}(h-h_m)}{1+Q^{(m,N_m+1-j)}(h)}, \end{cases} \end{cases} \tag{47}$$

for computing the continued fractions at fixed h

$$Q^{(1,1)}(h) = \left|S_1^{N_1}S_2^{N_2}\ldots S_K^{N_K}\right|_h \quad \text{or} \quad \left|S_1^{N_1}S_2^{N_2}\ldots S_K^{N_K}(V_{K,N_{K+1}})\right|_h, \tag{48}$$

from the input data

$$Q^{(K,N_K+1)}(h) = \begin{cases} 0 & \text{for } (48)_1, \\ V_{K,N_K}(h-h_K) & \text{for } (48)_2. \end{cases} \tag{49}$$

8. Numerical test

For the illustration of the Theorem 1 let us examine the following Stieltjes function

$$F(h) = 1+\ln[0.5(h+1)], \quad h \geq 0 \tag{50}$$

representing qualitatively the effective modulus $\lambda_e(h)/\lambda_1$ of the inhomogeneous media, cf. (2)–(3). The power expansions of $F(h)$ at K fixed points $h = h_m$ $(m = 1, 2, \dots, K)$ are given by

$$F_m(h - h_m) = \textstyle\sum_{n=o}^{\infty} F_{mn}(h - h_m)^n, \quad F_{m0} = 1 + \ln(0.5(h_m + 1)),$$
$$F_{mn} = (-1)^{n+1} \frac{(0.5)^n}{n[0.5(h_m + 1)]^n}, \quad n = 1, 2, \dots . \tag{51}$$

On account of (6), (7), (9), (22), (38) and (51), we obtain

$$f_m^{(1,1)}(h - h_m) = \sum_{n=0}^{\infty} f_{mn}^{(1,1)}(h - h_m)^n. \tag{52}$$

(i) If $h_m \neq 1$, then

$$f_{m0}^{(1,1)} = \frac{1}{h_m - 1}\Big[\, 1 + \ln[0.5(h_m + 1)] \,\Big],$$
$$f_{mn}^{(1,1)} = \frac{1}{h_m - 1}\Big[\, \frac{(0.5)^n}{n[0.5(h_m + 1)]^n} - f_{m(n-1)}^{(1,1)} \,\Big], \quad n = 1, 2, \dots k. \tag{53}$$

(ii) If $h_m = 1$, then

$$f_{mn}^{(1,1)} = \frac{(0.5)^{n+1}}{n + 1}, \quad n = 0, 1, \dots . \tag{54}$$

By applying the recurrence formulae (44)–(49) to the input data (52)–(54) we have evaluated the upper and lower bounds on the Stieltjes function $F(h) = 1 + \ln[0.5(h + 1)]$. The results are depicted in Figs. 1, 2 and Table 1.

9. Application

Prediction of the effective parameters from the given experimental data is one of the main tasks of the mechanics of inhomogeneous media. Theorem 1 derived in Section 4 jointly with multi-point

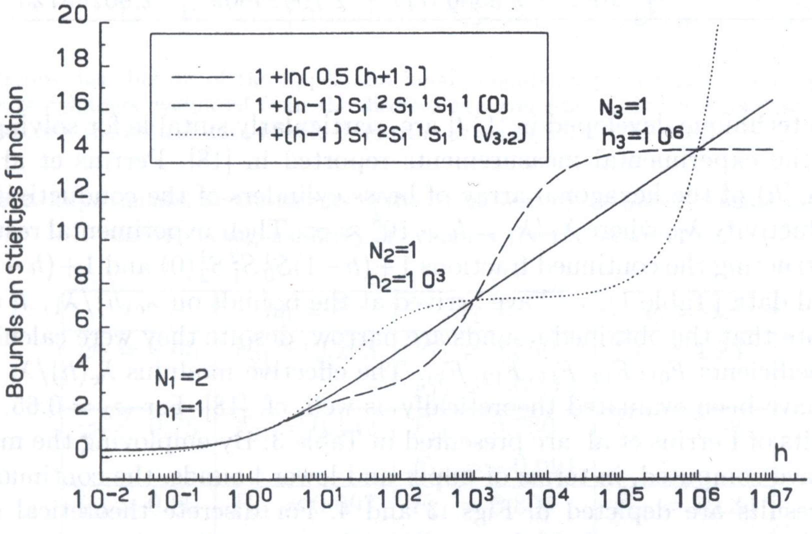

Fig. 1. Graphical illustration of the Theorem 1 for the parameters: $R = 0$, if $0 < h < 1$; $R = 2$, if $1 < h < 10^3$; $R = 3$, if $10^3 < h < 10^6$; $R = 4$, if $10^6 < h < \infty$.

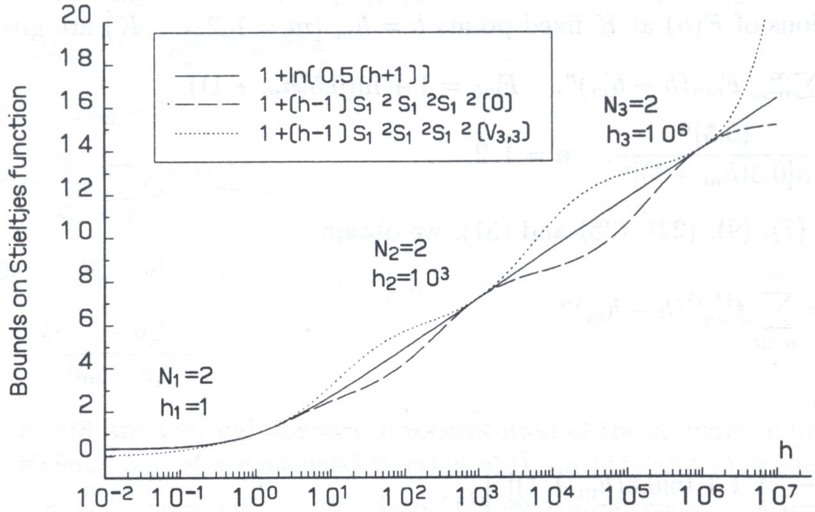

Fig. 2. Graphical illustration of the Theorem 1 for the parameters: $R = 0$, if $0 < h < 1$; $R = 2$, if $1 < h < 10^3$; $R = 4$, if $10^3 < h < 10^6$; $R = 6$, if $10^6 < h < \infty$.

Table 1. The best upper and lower bounds on $\ln(0.5(h+1))$ evaluated at $h_1 = 0.5$ and $h_2 = 1$ for a given N_1, N_2.

	h	$1+(h-1)$ $S_1^2S_1^1S_1^1(0)$	$\ln 0.5(h+1)$	$1+(h-1)$ $S_1^2S_1^1S_1^1(V_{4,2})$
	0.25	0.53330481	0.52999637	0.49470804
$N_1 = 1, N_2 = 1$	0.75	0.86623969	0.86646861	0.86801807
	10.0	2.34019024	2.70474809	4.64456884
	0.25	0.53018988	0.52999637	0.52754019
$N_1 = 2, N_2 = 1$	0.75	0.86648037	0.86646861	0.86640772
	10.0	3.06706375	2.70474809	2.39208456
	0.25	0.53001523	0.52999637	0.52960660
$N_1 = 2, N_2 = 2$	0.75	0.86646892	0.86646861	0.86646587
	10.0	2.63065777	2.70474809	2.96268723

Padé approximants technique developed in [1–3] are particularly suitable for solving that problem. Let us start from the experimental measurements reported in [18]. Perrins et al. measured the effective modulus $\lambda_e(h)$ of the hexagonal array of brass cylinders of the conductivity λ_2 immersed in water of the conductivity λ_1, where $\lambda_2/\lambda_1 = h > 10^8 \approx \infty$. Their experimental results are recalled in Table 2. By constructing the continued fractions $1+(h-1)S_0^1S_1^2S_2^1(0)$ and $1+(h-1)S_0^1S_1^2S_2^1(V_{2,2})$ for the experimental data (Table 1), we have arrived at the bounds on $\lambda_e(h)/\lambda_1$, $h \in (0,\infty)$ shown in Figs. 3 and 4. Note that the obtained bounds are narrow, despite they were calculated from only five power series coefficients $F_{01}, F_{10}, F_{11}, F_{12}, F_{30}$. The effective modulus $\lambda_e(h)/\lambda_1$ of a hexagonal array of cylinders have been evaluated theoretically as well, cf. [18]. For $\varphi_2 = 0.65$, 0.76 and 0.80, the theoretical results of Perrins et al. are presented in Table 3. By employing the multi-point Padé approximants we have computed, in terms of upper and lower bounds, the continuous distribution of $\lambda_e(h)/\lambda_1$. The results are depicted in Figs. 3 and 4. For discrete theoretical data (Table 3) the multi-point Padé approximants bounds coincide. They lay within the bounds evaluated from experimental data (Table 2).

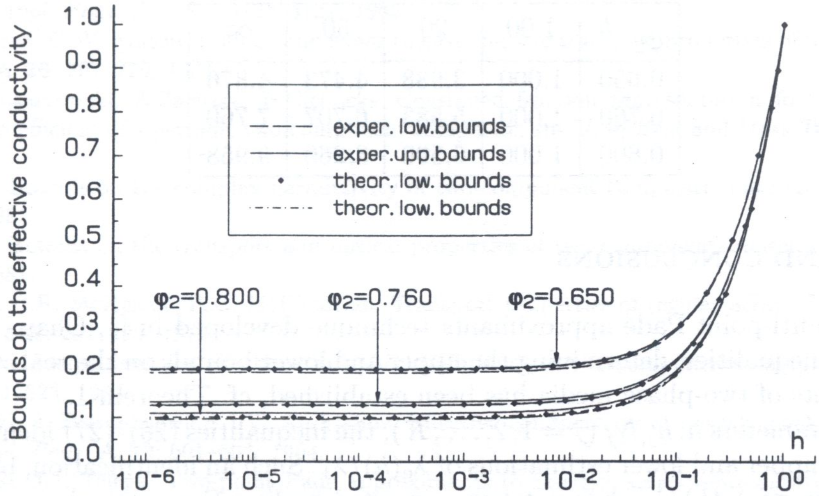

Fig. 3. Continuous distribution of the upper and lower bounds on the effective conductivity $\lambda_e(h)/\lambda_1$ of hexagonal array of cylinders evaluated from the discrete experimental measurements (Table 2, Perrins at al. 1979) and the discrete theoretical data (Table 3, Perrins at al. 1979), $0 < h < 1$.

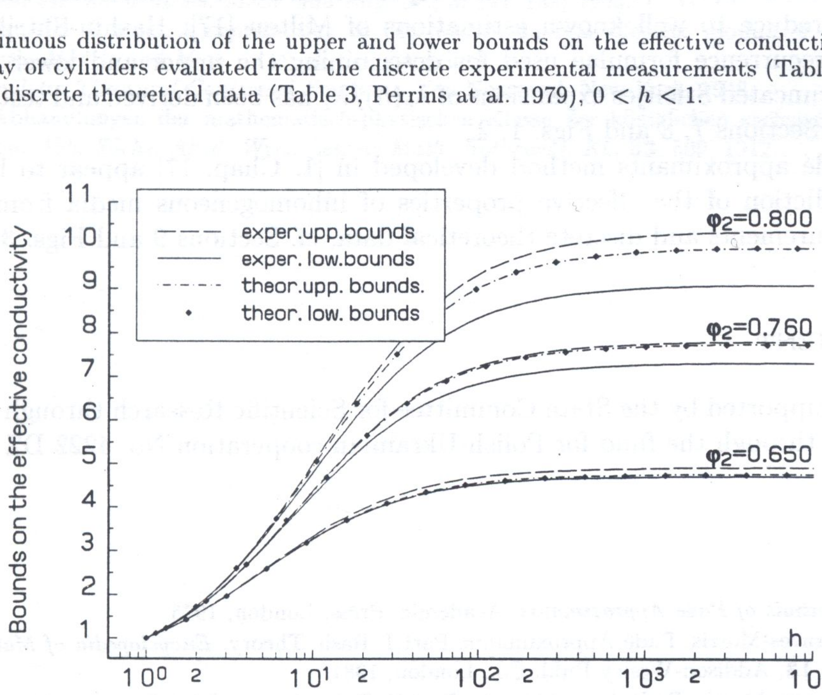

Fig. 4. Continuous distribution of the upper and lower bounds on the effective conductivity $\lambda_e(h)/\lambda_1$ of hexagonal array of cylinders evaluated from the discrete experimental measurements (Table 2, Perrins at al. 1979) and the discrete theoretical data (Table 3, Perrins at al. 1979), $1 < h < \infty$.

Table 2. Experimental measurements of the coefficients of the power expansion of λ_e/λ_1 for the hexagonal array of cylinders (Perrins et al.1979)

	$h_0 = 0$	$h_1 = 1$	$h_2 = \infty$
$\varphi_2 = 0.65$	$F_{01} = 0.203$	$F_{11} = 0.650$ $F_{12} = -0.114$	$F_{21} = 4.93$
$\varphi_2 = 0.75$	$F_{01} = 0.132$	$F_{11} = 0.760$ $F_{12} = -0.091$	$F_{21} = 7.58$
$\varphi_2 = 0.80$	$F_{01} = 0.097$	$F_{11} = 0.800$ $F_{12} = -0.08$	$F_{21} = 10.34$

Table 3. Values of $\lambda_e(h)/\lambda_1$ for a hexagonal array of cylinders evaluated theoretically by Perrins et al.1979

φ_2 \ h	1.00	20	50	∞
0.650	1.000	3.988	4.473	4.876
0.760	1.000	5.583	6.707	7.760
0.800	1.000	6.590	8.260	9.958

10. Summary and Conclusions

By applying the multi-point Padé approximants technique developed in [1, Chap. 17] the infinite set of new general inequalities, determining the upper and lower bounds on the real- valued effective transport coefficients of two-phase media has been established, cf. Theorem 1.

For the given parameters h, h_j, N_j $(j = 1, 2, \ldots, K)$, the inequalities (26)-(27) identify the bounds on $\lambda_e(h)/\lambda_1$ as the upper and lower estimations of $\lambda_e(h)/\lambda_1$. Such an identification, being important for the investigation of $\lambda_e(h)/\lambda_1$, has not been reported earlier. For particular cases the general bounds (26)-(27) reduce to well known estimations of Milton [17], Hashin-Shtrikman [13] and Wiener [24]. The recurrence formulae used for determining the upper and lower estimations of $\lambda_e(h)/\lambda_1$ from K truncated Stieltjes expansions of $\lambda_e(h)/\lambda_1$ has been derived and tested successfully for correctness, cf. Sections 7, 8 and Figs. 1, 2.

Multi-point Padé approximants method developed in [1, Chap. 17] appear to be particularly useful for the prediction of the effective properties of inhomogeneous media from the available experimental measurements and discrete theoretical data, cf. Sections 9 and Figs. 3, 4.

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References

[1] G.A. Baker. *Essentials of Padé Approximants.* Academic. Press, London, 1975.

[2] G.A. Baker, P. Graves-Morris. Padé Approximants. Part I: Basic Theory. *Encyclopedia of Mathematics and its Applications*, Vol. **13**, Addison-Wesley Publ. Co., London, 1981.

[3] G.A. Baker, P. Graves-Morris. Padé Approximants, Part II: Extensions and Applications. *Encyclopedia of Mathematics and its Applications*, Vol. **14**, Addison-Wesley Publ. Co., London, 1981.

[4] D.J. Bergman. The dielectric constant of a composite material — A problem in classical physics. *Phys. Report.* **C 43**: 377–407, 1978.

[5] D.J. Bergman. Bounds for the complex dielectric constants of two-component composite material. *Phys.Rev.* **B23, 6**: 3058–3065, 1981.

[6] D.J. Bergman. Rigorous bounds for the complex dielectric constants of a two-component composite material. *Ann.Phys.*, **138**: 78–114, 1982.

[7] D.J. Bergman. Hierarchies of Stieltjes functions and their applications to the calculation of bounds for the dielectric constant of a two-component composite medium. *SIAM J. Appl. Math.*, **53, 4**: 915–930, 1993.

[8] K.E. Clark, G.W. Milton. Optimal bounds correlating electric, magnetic and thermal properties of two-phase, two-dimensional composites. *Proc. Roy. Soc. London* A, **448**: 161–190, 1995.

[9] B.U. Felderhof. Bounds for the complex dielectric constant of a two-phase composite. *Physica* A, **126**: 430–442, 1984.

[10] J. Gilewicz. *Approximants de Padé.* Springer-Verlag, Berlin 1978.

[11] K. Golden and G. Papanicolaou. Bounds for effective parameters of heterogeneous media by analytic continuation. *Comm. Math. Phys.*, **90**: 473–491, 1983.

[12] K. Golden. Bounds on the complex permittivity of a multicomponent material. *J. Mech. Phys. Solids,* **34**: 333–358, 1986.

[13] Z. Hashin, S. Shtrikman. A variational approach to the theory of the effective magnetic permeability of multiphase materials. *J. Appl. Phys. Sol.*, **33**: 3125–3131, 1962.

[14] R.C. McPhedran, G.W. Milton. Bounds and exact theories for the transport properties of inhomogeneous media. *Appl. Phys.*, **A 26**: 207–220, 1981.

[15] S. May, S. Tokarzewski, A.Zachara, B.Cichocki. Continued fraction representation for the effective thermal conductivity coefficient of a periodic two-component composite. *Int. J. of Heat and Mass Transf.*, **37**: 2165–2173, 1994.

[16] G.W. Milton. Bounds on the complex permittivity of two-component composite material. *J.Appl.Phys.*, **52, 8**: 5288–5293, 1981.

[17] G.W. Milton. Bounds on the transport and optical properties of two-components material. *J. Appl. Phys.*, **52**: 5294–5304, 1981.

[18] W.T. Perrins, D.R. McKenzie, R.C. McPhedram. Transport properties of regular array of cylinders. *Proc. Roy. Soc. Lond. A* **369**: 207–225, 1979.

[19] S. Tokarzewski. Inequalities for effective transport coefficients of two-components composite materials. *Arch. Mech.*, **46**: 611–623, 1994.

[20] S. Tokarzewski, J. Bławzdziewicz, I.V. Andrianov. Effective conductivity of densely packed highly conducting cylinders. *Appl. Phys.* **A 59**: 601–604, 1994.

[21] S. Tokarzewski, J.J. Telega. Two-point Padé approximants to Stieltjes series representation of bulk moduli of regular composites. *Comp. Assis. Mech. and Eng. Sc.*, **3**: 121–132, 1996.

[22] S. Tokarzewski, J.J. Telega. A contribution to the bounds on real effective moduli of two-phase composite materials. *Math. Models and Meth. in Appl. Sci.* (in print).

[23] H.S. Wall. *Analytic Theory of Continued Fractions.* Van Nostrand, New York, 1948.

[24] O. Wiener. Abhandlungen der mathematisch-physischen Klasse der königlichen sachsischen Gesellschaft der Wissenschaften. *Abh. Sächs. Akad. Wiss. Leipzig Math.-Naturwiss. Kl.*, **32**: 509, 1912.