Multipoint matrix Padé approximant bounds on effective anisotropic transport coefficients of two-phase media

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Abstract. It is well known that a tensor Stieltjes function $\mathbf{f}$ represents an effective transport coefficient $\mathbf{q}$ of an inhomogeneous medium consisting of two isotropic components. In this paper, we investigate multipoint matrix Padé approximants to matrix expansions of $\mathbf{f}$. We prove that matrix Padé ones to $\mathbf{f}$ estimate $\mathbf{f}$ from the top and below. Consequently the Padé approximants to $\mathbf{q}$ form upper and lower bounds on $\mathbf{q}$. The inequalities for matrix Padé bounds on $\mathbf{f}$ and $\mathbf{q}$ are established. They reduce to the inequalities for scalar Padé ones Tokarzewski (ZAMP 61:773–780, 2010). As an illustrative example, matrix Padé estimates of an effective conductivity of a specially laminated two-phase medium are computed.

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1. Introduction

One of the most popular method of a calculation of effective physical properties $\mathbf{q}$ of inhomogeneous media is a method of bounds. Wiener [21] derived optimal bounds on $q_{jj}, j = 1, 2, 3$ with prescribed volume fractions. These bounds are known as the arithmetic and harmonic mean bounds. For isotropic materials, Hashin and Shtrikman [10] improved Wiener's bounds using variational principles. Bergman [3, 4] introduced a method for obtaining bounds on $q_{jj}, j = 1, 2, 3$ which does not rely on variational principles. Instead, he exploited the analyticity of $q_{jj}, j = 1, 2, 3$ as functions of the moduli of phases.

The method of Bergman was studied in more detail and applied to several physical problems by Milton [12–14, 17]. A rigorous justification of Bergman's approach is due to Golden and Papanicolaou [9]. Specific continued fraction techniques for an evaluation of bounds on $q_{jj}, j = 1, 2, 3$ were proposed by Bergman [5]. The last three authors recovered the bounds reported earlier in [11, 13].

Matrix continued fraction methods for computing matrix bounds on an effective, anisotropic transport coefficient $\mathbf{q}$ are reported in [6] and [17, Section 28.4], see also [15, 16]. Clark and Milton [6] calculate the matrix ones on $\mathbf{q}$ for two-dimensional composites only. They start from a power expansion of $\mathbf{q}(z)$ at $z = 0$ and the discrete values $\mathbf{q}(z_1), \mathbf{q}(z_2), \dots, \mathbf{q}(z_N)$. Milton [17, Section 28.4] deals mostly with three-dimensional composites. He computes the bounds on $\mathbf{q}$ from a power expansion of $\mathbf{q}(z)$ at $z = 0$. The aim of this paper is to establish multipoint matrix Padé bounds [1, 2] on an effective, anisotropic transport coefficient $\mathbf{q}$ of a two-phase medium for the case, when matrix power expansions of $\mathbf{q}$ at a number of real points are given.

1.1. Anisotropic transport coefficients as a matrix Stieltjes functions

The effective transport coefficient of a macroscopically anisotropic two-phase medium, say the thermal conductivity $\mathbf{q}$, is defined by

$$\frac{q_{jk}(z) - \delta_{jk}}{z} = \frac{1}{|Y|} \int_Y \Theta_2(y) \frac{\partial T^{(j)}(y)}{\partial y_k} dy, \quad z = h - 1, \quad h = \frac{\mu_2}{\mu_1}. \quad (1.1)$$

The temperature field $T^{(j)}(y)$ appearing in (1.1) satisfies the conductivity equation and periodic boundary conditions

$$\frac{\partial}{\partial y_k} \frac{\partial T^{(j)}(y)}{\partial y_k} + z \frac{\partial}{\partial y_k} \Theta_2(y) \frac{\partial T^{(j)}(y)}{\partial y_k} = 0, \quad (y_j - T^{(j)}) \text{ is } Y - \text{periodic}. \quad (1.2)$$

Here $\Theta_2(y)$ is a characteristic function of inclusions: $\Theta_2(y) = 1$ if $y \in \Theta_2$ and 0 otherwise. By μ_1 and μ_2 , we denote the thermal coefficients of a matrix and inclusions. The volume fraction is equal to $\varphi = \left(\int_Y \Theta_2(y) dy \right) / |Y|$, where Y is a unit cell. It is proved that the left-hand side of Eq. (1.1) is a matrix Stieltjes function [4, 9]

$$\mathbf{f}(z) = \frac{\mathbf{q}(z) - \mathbf{I}}{z} = \int_0^1 \frac{d\gamma(u)}{1 + zu}, \quad d\gamma(u) \geq \mathbf{0}, \quad z \in C \setminus [-\infty, -1) \quad (1.3)$$

satisfying the condition

$$\mathbf{f}(-1) \leq \mathbf{I}, \quad (1.4)$$

where $\mathbf{0}$ and $\mathbf{I}$ denote zero and unit matrices, respectively. The function defined by (1.3)–(1.4) we call a regular matrix Stieltjes one. Here the bold letters denote square matrices of order equal or more than two.

The aim of this paper is to establish upper and lower bounds on a matrix Stieltjes function $\mathbf{f}(z)$ (1.3)–(1.4) starting from the following partial information about $\mathbf{f}(z)$

$$\begin{aligned} \mathbf{f}(z) &= \sum_{i=0}^{p_j-1} \mathbf{c}_{ij} (z - z_j)^i + \mathbf{O}((z - z_j)^{p_j}), \quad z_j > -1, \quad j = 1, 2, \dots, N, \\ \mathbf{c}_{ij} &= \mathbf{c}_i(z_j) = \frac{\mathbf{f}^{(i)}(z_j)}{i!}, \quad \mathbf{f}^{(i)}(z_j) = \left. \frac{d^i \mathbf{f}(z)}{dz^i} \right|_{z=z_j}, \quad i = 0, 1, \dots, p_j - 1, \\ \mathbf{f}(-1) &= \mathbf{I}. \end{aligned} \quad (1.5)$$

Note that the inequality (1.4) is replaced by equality (1.5)₃. It is justified, since the bounds on $\mathbf{f}(z)$ incorporating the exact value $\mathbf{f}(-1) = \mathbf{C}$ ($\mathbf{0} \leq \mathbf{C} \leq \mathbf{I}$) are not worse than the ones incorporating $\mathbf{f}(-1) = \mathbf{I}$. Power expansions (1.5) we call regular multipoint matrix Stieltjes series.

The Keller–Dykhne–Mendelson relation reported in [6, Eq. (2.10)] imposes on a regular two-dimensional Stieltjes function $\mathbf{f}(z)$ (1.3) the following restriction

$$\mathbf{f}\left(-\frac{z}{z+1}\right) = \frac{z+1}{z} (\mathbf{I} - \mathbf{R}(1+z\mathbf{f}(z))^{-1}\mathbf{R}^T), \quad (1.6)$$

where $\mathbf{R}$ and $\mathbf{R}^T$ are the rotation matrices

$$\mathbf{R} = \begin{vmatrix} 0 & 1 \\ -1 & 0 \end{vmatrix}, \quad \mathbf{R}^T = \begin{vmatrix} 0 & -1 \\ 1 & 0 \end{vmatrix}. \quad (1.7)$$

The power expansions of $\mathbf{f}(z)$ at $z = z_j, j = 1, 2, \dots, N$ (1.5) determine via the equality (1.6) the power expansions of $\mathbf{f}(z)$ at $z = -\frac{z_j}{z_j+1}, j = 1, 2, \dots, N$

$$\mathbf{f}(z) = \sum_{i=0}^{p_j-1} \mathbf{c}_{ij} \left(z + \frac{z_j}{z_j+1}\right)^i + \mathbf{O}\left(\left(z + \frac{z_j}{z_j+1}\right)^{p_j}\right), \quad j = N+1, \dots, 2N. \quad (1.8)$$

From (1.6) and (1.8), we have at once:

Conclusion 1.1. *If the power expansions of $\mathbf{f}(z)$ at $z = z_j, j = 1, 2, \dots, N$ are given (1.5), then the power expansions of $\mathbf{f}(z)$ at $z = -\frac{z_j}{z_j+1}, j = 1, 2, \dots, N$ are known (1.8), provided that $\mathbf{f}(z)$ satisfy the Keller–Dykhne–Mendelson relation (1.6).*

On account of Conclusion 1.1, the methods working with the expansions (1.5) incorporate into Padé bounds on $\mathbf{f}(z)$ the Keller–Dykhne–Mendelson restriction (1.6) via the known expansions (1.8).

2. Matrix continued fractions to a matrix Stieltjes function

Now we apply a special transformation relating regular matrix Stieltjes series with matrix Stieltjes ones $\mathbf{f}_2(z)$ and $\mathbf{f}_3(z), \dots$, and $\mathbf{f}_{N+1}(z)$ as follows

$$\begin{aligned} \mathbf{f}_1(z) &= \epsilon_1 \frac{\mathbf{I}}{\mathbf{I} + (z - z_1)\mathbf{f}_2(z)} \epsilon_1, \quad \mathbf{f}_2(z) = \epsilon_2 \frac{\mathbf{I}}{\mathbf{I} + (z - z_2)\mathbf{f}_3(z)} \epsilon_2, \dots, \\ \mathbf{f}_j(z) &= \epsilon_j \frac{\mathbf{I}}{\mathbf{I} + (z - z_j)\mathbf{f}_{j+1}(z)} \epsilon_j, \quad \dots, \quad \mathbf{f}_N(z) = \epsilon_N \frac{\mathbf{I}}{\mathbf{I} + (z - z_N)\xi_{N+1}\varphi_{N+1}(z)\xi_{N+1}} \epsilon_N, \end{aligned} \quad (2.1)$$

where matrix coefficients ϵ_k and ξ_{N+1} are chosen in such a way that

$$\mathbf{f}_k(z_k) = \epsilon_k \epsilon_k, \quad k = 2, 3, \dots, N; \quad \varphi_{N+1}(-1) = \mathbf{I}. \quad (2.2)$$

Note that in formulae (2.1), the notation

$$\frac{\mathbf{I}}{\mathbf{I} + (z - z_j)\mathbf{f}_{j+1}(z)} = (\mathbf{I} + (z - z_j)\mathbf{f}_{j+1}(z))^{-1} \quad (2.3)$$

is introduced. Since $\mathbf{f}_1(z)$ is a regular matrix Stieltjes function from (2.1), we have

$$\begin{aligned} \mathbf{0} < \mathbf{f}_{k+1}(z_k), \quad \mathbf{0} < \mathbf{I} + (z - z_k)\mathbf{f}_{k+1}(z_k), \\ z_k > -1, \quad z > -1, \quad k = 1, 2, \dots, N. \end{aligned} \quad (2.4)$$

Recurrence relations (2.1) lead to a matrix continued fraction expansion of $\mathbf{f}_1(z)$ about N points $z_j, j = 1, 2, 3, \dots, N$

$$\mathbf{f}_1(z) = \epsilon_1 \overbrace{\hspace{10em}}^{\mathbf{I}} \epsilon_1. \quad (2.5)$$

$$\mathbf{I} + \epsilon_2 \overbrace{\hspace{10em}}^{(z - z_1)} \epsilon_2$$

$$\dots\dots\dots$$

$$\mathbf{I} + \epsilon_N \overbrace{\hspace{10em}}^{(z - z_{N-1})} \epsilon_N$$

$$\mathbf{I} + (z - z_N) \xi_{N+1} \varphi_{N+1}(z) \xi_{N+1}$$

It is convenient to rewrite (2.5) as follows

$$\mathbf{f}_1(z) = \epsilon_1 \frac{\mathbf{I}}{\mathbf{I} + (z - z_1)} \epsilon_1 \times \cdots \times \epsilon_N \frac{\mathbf{I}}{\mathbf{I} + (z - z_N)} \epsilon_N \times \xi_{N+1} \varphi_{N+1}(z) \xi_{N+1}, \quad (2.6)$$

or shortly

$$\mathbf{f}_1(z) = \bigvee_{k=1}^N \left(\epsilon_k \frac{\mathbf{I}}{\mathbf{I} + (z - z_k)} \epsilon_k \right) \times \xi_{N+1} \varphi_{N+1}(z) \xi_{N+1}. \quad (2.7)$$

Here the notation (2.3) is used.

3. Inequalities for matrix bounds on a matrix Stieltjes function

By substituting matrix Stieltjes series (1.5) to the recurrence relations (2.1), we obtain a general matrix continued fraction expansion of $\mathbf{f}_1(z)$

$$\mathbf{f}_1(z) = \bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \left(\epsilon_k \frac{\mathbf{I}}{\mathbf{I} + (z - z_k)} \epsilon_k \right) \times \xi_P \varphi_P(z) \xi_P, \\ P_0 = 0, \quad P_j = \sum_{i=1}^j p_i, \quad P = P_N + 1, \quad j = 1, 2, \dots, N. \quad (3.1)$$

Here $\varphi_P(z)$ is a regular matrix Stieltjes function. Hence it satisfies the restriction

$$\varphi_P(z) \in \phi_1(z) = \{\mathbf{u}; \mathbf{0} \leq \mathbf{u} \leq \mathbf{I}\}, \quad z \in [-1, \infty). \quad (3.2)$$

We call $\phi_1(z)$ the elementary inclusion region. The general inclusion one $\phi_P(z)$ is equal to

$$\mathbf{f}_1(z) \in \phi_P(z) = \{\mathbf{F}_P(z, \mathbf{u}); \mathbf{0} \leq \mathbf{u} \leq \mathbf{I}\}, \quad z \in [-1, \infty), \quad (3.3)$$

where (cf. (3.1)–(3.3))

$$\mathbf{F}_P(z, \mathbf{u}) = \bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \left(\epsilon_k \frac{\mathbf{I}}{\mathbf{I} + (z - z_k)} \epsilon_k \right) \times \xi_P (\mathbf{I} - \mathbf{u}) \xi_P. \quad (3.4)$$

In the “Appendix” we prove that two-dimensional Padé approximants $\mathbf{F}_P(z, \mathbf{u})$, $\mathbf{u} = \mathbf{0}, \mathbf{I}$ satisfy the Keller–Dykhne–Mendelson relation (cf. Conclusions 6.3)

$$\mathbf{F}_P \left(-\frac{z}{z+1}, \mathbf{u} \right) = \frac{z+1}{z} (\mathbf{I} - \mathbf{R}(\mathbf{I} + z\mathbf{F}_P(z, \mathbf{u}))^{-1} \mathbf{R}^T), \quad \mathbf{u} = \mathbf{0}, \mathbf{I}. \quad (3.5)$$

If $z \neq z_k$ and $\mathbf{u}_1 - \mathbf{u}_0 > \mathbf{0}$, then from (3.4) and (2.4), it follows

$$\mathbf{F}_P(z, \mathbf{u}_1) - \mathbf{F}_P(z, \mathbf{u}_0) < \mathbf{0} \text{ or } \mathbf{F}_P(z, \mathbf{u}_1) - \mathbf{F}_P(z, \mathbf{u}_0) > \mathbf{0}. \quad (3.6)$$

This means that the following relations (cf. (3.3))

$$\mathbf{f}_1(z) \in \phi_P(z) < \phi_{P-1}(z) < \dots < \phi_2(z) < \phi_1(z). \quad (3.7)$$

are satisfied. From (3.7), we have

Conclusion 3.1. *The matrix Stieltjes function $\mathbf{f}_1(z)$ lies between matrix Padé approximants $\mathbf{F}_P(z, \mathbf{0})$ and $\mathbf{F}_P(z, \mathbf{I})$. The Padé ones $\mathbf{F}_P(z, \mathbf{0})$ and $\mathbf{F}_P(z, \mathbf{I})$ form the best estimates of $\mathbf{f}_1(z)$ obtainable using only the given P power series coefficients, and that the use of additional power series ones (higher P) improves the bounds $\mathbf{F}_P(z, \mathbf{0})$ and $\mathbf{F}_P(z, \mathbf{I})$ on $\mathbf{f}_1(z)$.*

The question arises, which expression $\mathbf{F}_P(z, \mathbf{0})$ or $\mathbf{F}_P(z, \mathbf{I})$ gives the upper bound, and which gives the lower one on $\mathbf{f}_1(z)$. To answer this question, we fix z

$$z_M < z < z_{M+1}, \quad z_1 < z_2 < \dots < z_M < z_{M+1} < \dots < z_N \quad (3.8)$$

and split continued fractions (3.1) and (3.4) into two parts

$$\mathbf{f}_1(z) = \times \bigvee_{k=1}^M \bigvee_{j=P_{k-1}+1}^{P_k} \left(\epsilon_k \frac{\mathbf{I}}{\mathbf{I} + (z - z_k)} \epsilon_k \right) \times \\ \times \bigvee_{k=N-M+1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \left(\epsilon_k \frac{\mathbf{I}}{\mathbf{I} + (z - z_k)} \epsilon_k \right) \times \xi_P \varphi_P(z) \xi_P \quad (3.9)$$

and

$$\begin{aligned} \mathbf{F}_P(z, \mathbf{0}) &= \bigvee_{k=1}^M \bigvee_{j=P_{k-1}+1}^{P_k} \left(\epsilon_k \frac{\mathbf{I}}{\mathbf{I} + (z - z_k)} \epsilon_k \right) \times \\ &\times \bigvee_{k=N-M+1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \left(\epsilon_k \frac{\mathbf{I}}{\mathbf{I} + (z - z_k)} \epsilon_k \right) \times \xi_P \mathbf{I} \xi_P. \end{aligned} \quad (3.10)$$

Due to (3.6), the second part of (3.10) is greater in a matrix sense than the second one of (3.9). Hence the calculation of the first parts of (3.9) and (3.10) yield the inequality (cf. [8, 20])

$$(-1)^{L_P(z)} \mathbf{F}_P(z, \mathbf{0}) \leq (-1)^{L_P(z)} \mathbf{f}_1(z) \quad (3.11)$$

leading to the fundamental ones (cf. Conclusion 3.1)

$$\begin{aligned} (-1)^{L_P(z)} \mathbf{F}_P(z, \mathbf{0}) &\leq (-1)^{L_P(z)} \mathbf{f}_1(z) \leq (-1)^{L_P(z)} \mathbf{F}_P(z, \mathbf{I}), \\ L_P(z) &= \sum_{j=1}^N p_j H(z - z_j) + 1, \\ H(z) &= 0 \text{ if } z < 0 \text{ or } H(z) = 1 \text{ if } z \geq 0. \end{aligned} \quad (3.12)$$

Here $L_P(z)$ depends on the input parameters p_j, z_j , see (1.5). We call $L_P(z)$ the input function. It is easy to check that matrix inequalities (3.12) reduce to the scalar ones reported in [19, (2.11)–(2.12)].

4. Fundamental inequalities for matrix bounds on effective transport coefficients

It is convenient to rewrite (1.3) as follows

$$\mathbf{f}_1(z) = \frac{\mathbf{Q}(z)}{z}, \quad \mathbf{Q}(z) = \mathbf{q}(z) - \mathbf{I}. \quad (4.1)$$

Here $\mathbf{q}(z)$ is an anisotropic effective transport coefficient. Due to (4.1)₁, the inequalities (3.12) take two equivalent forms (cf. (4.1))

$$\begin{aligned} (-1)^{L_P(z)} \mathbf{F}_P(z, \mathbf{0}) &\leq (-1)^{L_P(z)} \frac{\mathbf{Q}(z)}{z} \leq (-1)^{L_P(z)} \mathbf{F}_P(z, \mathbf{I}), \\ L_P(z) &= \sum_{j=1}^N p_j H(z - z_j) + 1, \end{aligned} \quad (4.2)$$

or

$$\begin{aligned} (-1)^{R_P(z)} z \mathbf{F}_P(z, \mathbf{0}) &\geq (-1)^{R_P(z)} \mathbf{Q}(z) \geq (-1)^{R_P(z)} z \mathbf{F}_P(z, \mathbf{I}), \\ R_P(z) &= L_P(z) + H(z). \end{aligned} \quad (4.3)$$

The formulae (4.3) determine, in terms of input parameters z_j, p_j , the upper and lower bounds on an effective, anisotropic transport coefficients $\mathbf{Q}(z)$ of a two-phase medium. For isotropic composites, the matrix inequalities (4.3) reduce to the scalar ones reported in [19, (3.3)].

4.1. Illustrative example

In order to illustrate the inequalities obtained, we consider a matrix Stieltjes function

$$\mathbf{f}_1(z) = \begin{bmatrix} \frac{32 + 38z + 9z^2}{64 + 96z + 38z^2 + 3z^3} & -\frac{2(1+z)\sqrt{3}z}{64 + 96z + 38z^2 + 3z^3} \\ -\frac{2(1+z)\sqrt{3}z}{64 + 96z + 38z^2 + 3z^3} & \frac{3z^3 + 128 + 168z + 52z^2}{4(64 + 96z + 38z^2 + 3z^3)} \end{bmatrix}. \quad (4.4)$$

representing the effective transport coefficient $\mathbf{Q}(z)$ of a specially laminated two-phase material. The power expansion of (4.4) at $z = 0$ is given by

$$\mathbf{f}_1(z) = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} - \begin{bmatrix} \frac{5}{32} & \frac{1}{32}\sqrt{3} \\ \frac{1}{32}\sqrt{3} & \frac{3}{32} \end{bmatrix} z + \begin{bmatrix} O & O \\ O & O \end{bmatrix} (z^2). \quad (4.5)$$

Here we have (cf. (4.4))

$$\mathbf{f}_1(-1) \leq \mathbf{I}. \quad (4.6)$$

The input function (3.12) and the bounding one (3.4) reduce to (cf. (4.6))

$$L_3(z) = H(z+1) + 2H(z) \quad (4.7)$$

and (cf. (4.5)–(4.6))

$$\mathbf{F}_3(z, \mathbf{u}) = \epsilon_1 \frac{\mathbf{I}}{\mathbf{I} + \epsilon_2 \frac{z}{\mathbf{I} + z\xi_3(\mathbf{I} - \mathbf{u})\xi_3}} \epsilon_1, \quad (4.8)$$

where (cf. recurrence formula (2.1))

$$\epsilon_1 = \begin{bmatrix} -0.70710678 & +0.00000000 \\ +0.00000000 & -0.70710678 \end{bmatrix}, \quad \epsilon_2 = \begin{bmatrix} -0.37089098 & -0.41825815 \\ -0.41825815 & +0.11207193 \end{bmatrix} \quad (4.9)$$

and

$$\xi_3 = \begin{bmatrix} -0.1584936486 & -0.5915063507 \\ -0.5915063507 & +0.5245190531 \end{bmatrix}. \quad (4.10)$$

From (4.5) to (4.6) and (3.12), it follows the inequalities

$$\mathbf{F}_3(z, \mathbf{0}) \geq \mathbf{f}_1(z) \geq \mathbf{F}_3(z, \mathbf{I}), \quad z \in [-1, \infty). \quad (4.11)$$

They impose on the components of matrices $\mathbf{F}_3(z, \mathbf{0})$, $\mathbf{f}_1(z)$, $\mathbf{F}_3(z, \mathbf{I})$ the restrictions

$$\begin{aligned} F_3(z, 0)_{jj} &\geq f_1(z)_{jj} \geq F_3(z, 1)_{jj}, \quad j = 1, 2, \\ -\sqrt{\Delta_3} + F_3(z, 0)_{12} &\leq f_1(z)_{12} \leq \sqrt{\Delta_3} + F_3(z, 0)_{12}, \\ -\sqrt{\Delta_3} + F_3(z, 1)_{12} &\leq f_1(z)_{12} \leq \sqrt{\Delta_3} + F_3(z, 1)_{12}, \end{aligned} \quad (4.12)$$

where

$$\Delta_3 = (F_3(z, 0)_{11} - F_3(z, 1)_{11})(F_3(z, 0)_{22} - F_3(z, 1)_{22}). \quad (4.13)$$

Definition 4.1. Estimates $\mathbf{F}_3(z, \mathbf{0})$ and $\mathbf{F}_3(z, \mathbf{I})$ satisfying (4.11), we call matrix Padé bounds on a matrix Stieltjes function (4.4).

Now we consider diagonal components of a matrix power expansion of $\mathbf{f}_1(z)$ only (cf. (4.5))

$$f_1(z)_{11} = \frac{1}{2} - \frac{5}{32}z + O(z^2), \quad f_1(z)_{22} = \frac{1}{2} - \frac{3}{32}z + O(z^2). \quad (4.14)$$

FIG. 1. **a** Scalar (solid lines) and matrix (boxes) Padé bounds on diagonal component $f_1(z)_{11}$ (dashed line) of a matrix Stieltjes function (4.4); **b** Differences between Padé bounds: upper scalar and upper matrix (solid line with empty boxes); lower scalar and lower matrix (solid line with solid boxes)

FIG. 2. **a** Scalar (solid lines) and matrix (boxes) Padé bounds on component $f_1(z)_{12}$ (dashed line) of a matrix Stieltjes function (4.4); **b** Differences between Padé bounds: upper scalar and upper matrix (solid line with empty boxes); lower scalar and lower matrix (solid line with solid boxes)

The bounding functions $F_3^s(z, u)_{11}$ and $F_3^s(z, u)_{22}$ constructed to (4.14) take the forms (cf. [19, (1.6)])

$$F_3^s(z, u)_{11} = \frac{\frac{1}{2}}{1 + \frac{z \frac{5}{16}}{1 + z \frac{3}{8}(1-u)}}, \quad F_3^s(z, u)_{22} = \frac{\frac{1}{2}}{1 + \frac{z \frac{3}{16}}{1 + z \frac{5}{8}(1-u)}}. \quad (4.15)$$

They estimate $f_1(z)_{ij}$ as follows (cf. ([19, (2.11)–(2.12)]))

$$\begin{aligned} F_3^s(z, 0)_{jj} \geq f_1(z)_{jj} \geq F_3^s(z, 1)_{jj}, \quad j = 1, 2, \quad z \in [-1, \infty), \\ -F_3^s(z, 1)_{12} \leq f_1(z)_{12} \leq +F_3^s(z, 1)_{12}, \end{aligned} \quad (4.16)$$

where

$$F_3^s(z, 1)_{12} = \sqrt{F_3^s(z, 1)_{11} F_3^s(z, 1)_{22}}. \quad (4.17)$$

Definition 4.2. Bounds $F_3^s(z, 0)_{ij}$ and $F_3^s(z, 1)_{ij}$, $j = 1, 2$ fulfilling (4.16)–(4.17), we call scalar Padé ones on a matrix Stieltjes function (4.4).

Scalar Padé bounds $F_3^s(z, 0)_{jj}$ and $F_3^s(z, 1)_{jj}$ are the Padé approximants to matrix Padé ones $F_3(z, 0)_{jj}$ and $F_3(z, 1)_{jj}$, respectively. Therefore, they satisfy the inequalities

$$F_3^s(z, 0)_{jj} \geq F_3(z, 0)_{jj} \text{ and } F_3^s(z, 1)_{jj} \geq F_3(z, 1)_{jj}, \quad j = 1, 2 \quad (4.18)$$

writing, matrix Padé bounds (4.12)–(4.13) are not worse than scalar Padé ones (4.16)–(4.17).

Numerical calculations of scalar and matrix Padé bounds on a matrix Stieltjes function $\mathbf{f}_1(z)$ and an effective transport coefficient $\mathbf{Q}(z)$ are carried out and compared with the exact test functions $\mathbf{f}_1(z)$ and $z\mathbf{f}_1(z)$ given by (4.4). The Padé estimates of $\mathbf{f}_1(z)$ and $\mathbf{Q}(z)$ are depicted in Figs. 1, 2, 3, 4, 5 and 6. Note that the bounds $F_3^s(z, 0)_{ij}$, $F_3^s(z, 1)_{ij}$, $F_3(z, 0)_{ij}$, $F_3(z, 1)_{ij}$ and $zF_3^s(z, 0)_{ij}$, $zF_3^s(z, 1)_{ij}$, $zF_3(z, 0)_{ij}$, $zF_3(z, 1)_{ij}$, $i, j = 1, 2$ satisfy the inequalities (4.12), (4.16) and (4.18), respectively. The matrix Padé bounds $\mathbf{F}_3(z, \mathbf{0})$ and $\mathbf{F}_3(z, \mathbf{I})$ given by (4.8)–(4.10) fulfil the Keller–Dykhne–Mendelson restriction (1.6).

FIG. 3. **a** Scalar (*solid lines*) and matrix (*boxes*) Padé bounds on diagonal component $f_1(z)_{22}$ (*dashed line*) of a matrix Stieltjes function (4.4); **b** Differences between Padé bounds: upper scalar and upper matrix (*solid line with empty boxes*); lower scalar and lower matrix (*solid line with solid boxes*)

FIG. 4. **a** Scalar (*solid lines*) and matrix (*boxes*) Padé bounds on diagonal component $Q(z)_{11}$ (*dashed line*) of a transport coefficient $Q(z)$; **b** Differences between Padé bounds: upper scalar and upper matrix (*solid line with empty boxes*); lower scalar and lower matrix (*solid line with solid boxes*)

FIG. 5. **a** Scalar (*solid lines*) and matrix (*boxes*) Padé bounds on a component $Q(z)_{12}$ (*dashed line*) of a transport coefficient $Q(z)$; **b** Differences between Padé bounds: upper scalar and upper matrix (*solid line with empty boxes*); lower scalar and lower matrix (*solid line with solid boxes*)

FIG. 6. **a** Scalar (*solid lines*) and matrix (*boxes*) Padé bounds on a component $Q(z)_{22}$ (*dashed line*) of a transport coefficient $Q(z)$; **b** Differences between Padé bounds: upper scalar and upper matrix (*solid line with empty boxes*); lower scalar and lower matrix (*solid line with solid boxes*)

5. Conclusions and final remarks

In order to predict which an estimate $z\mathbf{F}_P(z, \mathbf{0})$ or $z\mathbf{F}_P(z, \mathbf{I})$ gives an upper bound and which gives a lower one on an effective tensor $\mathbf{Q}(z)$, the fundamental inequalities for matrix Padé approximants $z\mathbf{F}_P(z, \mathbf{0})$ and $z\mathbf{F}_P(z, \mathbf{I})$ to an effective transport coefficient $\mathbf{Q}(z)$ are derived, see (4.3). The inequalities obtained generalize the previous scalar ones reported by Wiener [21], Hashin and Shtrikman [10], Milton [17] and Tokarzewski [18, 19].

It is developed a multipoint matrix continued fraction method (MMCFM) for computing multipoint matrix Padé bounds $z\mathbf{F}_P(z, \mathbf{0})$ and $z\mathbf{F}_P(z, \mathbf{I})$ on an effective, anisotropic transport coefficient $\mathbf{Q}(z)$, see ((2.1)–(2.7)). MMCFM incorporates into $z\mathbf{F}_P(z, \mathbf{0})$ and $z\mathbf{F}_P(z, \mathbf{I})$ the matrix coefficients of power expansions of $\mathbf{f}(z)$ at a number of real points.

The bounds $z\mathbf{F}_P(z, \mathbf{0})$ and $z\mathbf{F}_P(z, \mathbf{I})$ are the best with respect to the given power series coefficients (1.6) and (1.8). An additional restriction on $\mathbf{f}(z)$ (for example the Keller–Dykhne–Mendelson relation (3.5)) added to the given ones (1.6) and (1.8) allows us to improve the elementary inclusion region (3.2) and thus to improve the bounds $z\mathbf{F}_P(z, \mathbf{0})$ and $z\mathbf{F}_P(z, \mathbf{I})$ (3.4). Now we are working on this problem.

In order to illustrate MMCFM, the bounds $z\mathbf{F}_3(z, \mathbf{0})$ and $z\mathbf{F}_3(z, \mathbf{I})$ on two-dimensional $\mathbf{Q}(z)$ are calculated. As an input data, we take two coefficients of power expansions of $\mathbf{f}(z)$ at $z = 0$, see (4.5). Numerical values of $\mathbf{F}_3(z, \mathbf{u})$ and $z\mathbf{F}_3(z, \mathbf{u})$, $\mathbf{u} = \mathbf{0}, \mathbf{I}$ depicted in Figs. 1, 2, 3, 4, 5 and 6 confirm the inequalities (4.2)–(4.3).

MMCFM is especially suited for various implementations as a fast, accurate, numerical algorithm (2.1)–(2.7), since it is simply recursive and does not involve the solutions of a large number of equations or the computation of the zeros of high-degree polynomials. It can be used for an investigation of an inverse homogenization problem studied in [7, 22].

6. Appendix

Let us rewrite the K–D–M relation (1.6) as follows

$$\frac{1}{z+1}\mathbf{f}\left(-\frac{z}{z+1}\right) = \frac{1}{z}(\mathbf{I} - \mathbf{R}(\mathbf{I} + z\mathbf{f}(z))^{-1}\mathbf{R}^T). \quad (6.1)$$

Assume that $\mathbf{f}(z)$ appearing in (6.1) is a matrix Stieltjes function defined by (1.3)–(1.4). Let the matrix values of $\mathbf{f}(z)$ at $\frac{N}{2}$ real points be given

$$\mathbf{f}(z_{2j-1}), \quad j = 1, 2, \dots, \frac{N}{2}, \quad N\text{-even number}. \quad (6.2)$$

The $\frac{N}{2}$ values of $\mathbf{f}(-\frac{z}{z+1})$, $z \neq 0$ follow from the K–D–M equality (6.1) and the input data (6.2)

$$\mathbf{f}(z_{2j}) = \frac{z_{2j-1} + 1}{z_{2j-1}}(\mathbf{I} - \mathbf{R}(\mathbf{I} + z_{2j-1}\mathbf{f}(z_{2j-1}))^{-1}\mathbf{R}^T), \quad j = 1, 2, \dots, \frac{N}{2}. \quad (6.3)$$

The multipoint matrix Padé approximants $\mathbf{L}_N(z)$ to the discrete values (6.2)–(6.3) take the form (cf. (2.6))

$$\mathbf{L}_N(z) = \epsilon_1 \frac{\mathbf{I}}{\mathbf{I} + (z - z_1)} \epsilon_1 \times \dots \times \epsilon_{N-1} \frac{\mathbf{I}}{\mathbf{I} + (z - z_{N-1})} \epsilon_{N-1} \times \epsilon_N \epsilon_N. \quad (6.4)$$

Here the matrix coefficients ϵ_j satisfy the fitting equations

$$\mathbf{L}_N(z_j) = \mathbf{f}(z_j), \quad j = 1, 2, \dots, N. \quad (6.5)$$

Theorem 6.1. *If a matrix Stieltjes function $\mathbf{f}(z)$ (1.3)–(1.4) satisfies the K–D–M relation (6.1), then the multipoint matrix Padé approximants $\mathbf{L}_N(z)$ (6.4)–(6.5) to the known discrete values of $\mathbf{f}(z)$ (6.2)–(6.3) also satisfy the K–D–M relation (6.1), that is,*

$$\frac{1}{z+1}\mathbf{L}_N\left(-\frac{z}{z+1}\right) = \frac{1}{z}(\mathbf{I} - \mathbf{R}(\mathbf{I} + z\mathbf{L}_N(z))^{-1}\mathbf{R}^T). \quad (6.6)$$

Proof. Let us introduce the functions $\mathbf{U}_N(z)$ and $\mathbf{V}_N(z)$ depending on $\mathbf{L}_N(z)$ as follows (cf. the K–D–M equality (6.6))

$$\mathbf{U}_N(z) = \frac{1}{z+1}\mathbf{L}_N\left(-\frac{z}{z+1}\right) \quad \text{and} \quad \mathbf{V}_N(z) = \frac{1}{z}(\mathbf{I} - \mathbf{R}(\mathbf{I} + z\mathbf{L}_N(z))^{-1}\mathbf{R}^T). \quad (6.7)$$

From a recurrence formula for (6.4), it follows that $\mathbf{U}_N(z)$ and $\mathbf{V}_N(z)$ possess matrix continued fraction representations

$$\mathbf{U}_N(z) = \bigvee_{k=1}^{N-1} \left(\tau_k \frac{\mathbf{I}}{\mathbf{I} + (z - z_k)} \tau_k \right) \times^{\tau_N \tau_N}, \quad \tau_k \tau_k > 0 \quad (6.8)$$

and

$$\mathbf{V}_N(z) = \bigvee_{k=1}^{N-1} \left(\gamma_k \frac{\mathbf{I}}{\mathbf{I} + (z - z_k)} \gamma_k \right) \times^{\gamma_N \gamma_N}, \quad \gamma_k \gamma_k > 0, \quad (6.9)$$

where τ_j and $\gamma_j, j = 1, 2, \dots, N$ are real matrix coefficients. The relations (6.1)–(6.5) impose on (6.8)–(6.9) the restrictions $\mathbf{U}_N(z_j) = \mathbf{V}_N(z_j), j = 1, 2, \dots, N$, that is,

$$\bigvee_{k=1}^{N-1} \left(\tau_k \frac{\mathbf{I}}{\mathbf{I} + (z_j - z_k)} \tau_k \times^{\tau_N \tau_N} \right) = \bigvee_{k=1}^{N-1} \left(\gamma_k \frac{\mathbf{I}}{\mathbf{I} + (z_j - z_k)} \gamma_k \right) \times^{\gamma_N \gamma_N}. \quad (6.10)$$

The system of equations (6.10) yield at once

$$\tau_j = \gamma_j, \quad j = 1, 2, \dots, N. \quad (6.11)$$

On account (6.7)–(6.9) and (6.11) we obtain (6.6) immediately. $\square$

Let us consider now the additional restriction (cf. (1.4))

$$\mathbf{f}(z_{N+1}) = \mathbf{f}(-1) = \mathbf{I}. \quad (6.12)$$

Matrix Padé approximants $\mathbf{L}_{N+1}(z)$ to the input data (6.2)–(6.3) and (6.12) take the forms (cf. (6.4))

$$\mathbf{L}_{N+1}(z) = \epsilon_1 \frac{\mathbf{I}}{\mathbf{I} + (z - z_1)} \epsilon_1 \times \dots \times \epsilon_N \frac{\mathbf{I}}{\mathbf{I} + (z - z_{N-1})} \epsilon_N \times \xi_{N+1} \xi_{N+1}, \quad (6.13)$$

where (cf. (6.2)–(6.3))

$$\mathbf{L}_{N+1}(z_j) = \mathbf{f}(z_j), \quad j = 1, 2, \dots, N+1. \quad (6.14)$$

Since $\epsilon_j \epsilon_j > 0, j = 1, 2, \dots, N$ and $\xi_{N+1} \xi_{N+1} > 0$ from (6.13), it follows that

$$\mathbf{L}_{N+1}(\infty) > 0, \text{ if } N \text{ is even.} \quad (6.15)$$

Now we are prepared to prove:

Theorem 6.2. *If a matrix Stieltjes function $\mathbf{f}(z)$ (1.3)–(1.4) satisfies the K–D–M relation (6.1), then the multipoint matrix Padé approximants $\mathbf{L}_{N+1}(z)$ (6.13) to discrete values (6.2)–(6.3) and (6.12) also satisfy the K–D–M relation (6.1), that is,*

$$\mathbf{L}_{N+1} \left(-\frac{z}{z+1} \right) = \frac{z+1}{z} (\mathbf{I} - \mathbf{R}(\mathbf{I} + z\mathbf{L}_{N+1}(z))^{-1} \mathbf{R}^T). \quad (6.16)$$

Proof. Due to (6.12) and (6.15) at $z = \infty, -1$, the matrix approximants $\mathbf{L}_{N+1}(z)$ satisfy the K–D–M relation (6.16)

$$\left(\mathbf{L}_{N+1} \left(-\frac{z}{z+1} \right) \right)_{\infty, -1} = \left(\frac{z+1}{z} (\mathbf{I} - \mathbf{R}(\mathbf{I} + z\mathbf{L}_{N+1}(z))^{-1} \mathbf{R}^T) \right)_{\infty, -1} \quad (6.17)$$

Moreover, we also have (cf. (6.2)–(6.3) and (6.14))

$$\left(\mathbf{L}_{N+1} \left(-\frac{z}{z+1} \right) \right)_{z_1, z_2, \dots, z_N} = \left(\frac{z+1}{z} (\mathbf{I} - \mathbf{R}(\mathbf{I} + z\mathbf{L}_{N+1}(z))^{-1} \mathbf{R}^T) \right)_{z_1, z_2, \dots, z_N} \quad (6.18)$$

Note that for $z = -1, z_1, z_2, \dots, z_N, \infty$ the equalities (6.17)–(6.18) are true. On account of Theorems 6.1 and 6.2, they are also true for arbitrary z , see (6.16). $\square$

In order to illustrate Theorems 6.1 and 6.2, we consider the elementary matrix Padé bounds on $\mathbf{f}(z)$

$$\mathbf{L}_0(z) = \mathbf{0} \leq \mathbf{f}(z) \leq \mathbf{L}_1(z) = \mathbf{I}. \quad (6.19)$$

It is easy to check that $\mathbf{L}_0(z)$ and $\mathbf{L}_1(z)$ appearing in (6.19) satisfy the K–D–M relation (6.16). From (6.19) and (1.3), it follows the matrix bounds on an effective coefficient $\mathbf{q}(z)$

$$\mu_1 \mathbf{I} \leq \mathbf{q}(z) \leq \mu_2 \mathbf{I} \text{ leading to } \mu_1 \leq \lambda_1(z), \lambda_2(z) \leq \mu_2. \quad (6.20)$$

where μ_1, μ_2 are transport properties of components of a composite material, while $\lambda_1(z), \lambda_2(z)$ denote the eigenvalues of an effective coefficient $\mathbf{q}(z)$. It is worth noting that the bounds (6.20)₂ satisfy the inequalities [6, Ineq.(9.7)].

Since Theorems 6.1 and 6.2 are valid for any sets of discrete values of $\mathbf{f}(z)$ surrounding the fixed ones $\mathbf{f}(z_j)$, $j = 1, 2, \dots, N$ they are also valid for power expansions of $\mathbf{f}(z)$ at z_j , $j = 1, 2, \dots, N$. On account of that we conclude:

Conclusion 6.3. *If a matrix Stieltjes function $\mathbf{f}(z)$ (1.3)–(1.4) satisfies the K–D–M relation (1.6), then the multipoint matrix Padé approximants $\mathbf{F}_P(z, \mathbf{I})$ and $\mathbf{F}_P(z, \mathbf{0})$ (3.4) to matrix power expansions ((1.5)_{1,2}, (1.8)) and ((1.5)_{1,2,3}, (1.8)) also satisfy the K–D–M relation (1.6).*

$$\mathbf{F}_P(z, \mathbf{u}) \left(-\frac{z}{z+1} \right) = \frac{z+1}{z} (\mathbf{I} - \mathbf{R}(\mathbf{I} + z\mathbf{F}_P(z, \mathbf{u}))^{-1} \mathbf{R}^T), \quad \mathbf{u} = \mathbf{0}, \mathbf{I}. \quad (6.21)$$

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References

1. Baker, G. Jr.: Best error bounds for Padé approximants to convergent series of Stieltjes. J. Math. Phys. **10**(5), 814–820 (1969)
2. Baker, G. Jr.: Essentials of Padé Approximants. Academic Press, New York (1975)
3. Bergman, D.J.: Variational bounds on some bulk properties of two-phase composite material. Phys. Rev. B (Solid State) **14**, 1531–1542 (1976)
4. Bergman, D.J.: The dielectric constant of a composite material—a problem in classical physics. Phys. Rep. C **43**, 377–407 (1978)
5. Bergman, D.J.: Hierarchies of Stieltjes functions and their application to the calculation of bounds for the dielectric constant of a two-components composite medium. SIAM J. Appl. Math. **53**(4), 915–930 (1993)
6. Clark, K.E., Milton, G.W.: Optimal bounds correlating electric, magnetic and thermal properties of two-phase, two-dimensional composites. Proc. Roy. Soc. Lond. A **448**, 161–190 (1995)
7. Cherkaev, E.: Inverse homogenization with diagonal Padé approximants. PAMM **7**, 10420001–1042002 (2007)
8. Gilewicz, J., Pindor, M., Telega, J.J., Tokarzewski, S.: N-point Padé approximants and two sided estimates of errors on the real axis for Stieltjes functions. J. Comput. Appl. Math. **178**, 247–253 (2005)
9. Golden, K., Papanicolaou, G.: Bounds for effective parameters of heterogeneous media by analytic continuation. Commun. Math. Phys. **90**(4), 473–491 (1983)
10. Hashin, Z., Shtrikman, S.: A variational approach to the theory of the effective magnetic permeability of multiphase materials. J. Appl. Phys. Sol. **33**, 3125–3131 (1962)
11. McPhedran, R.C., Milton, G.W.: Bounds and exact theories for the transport properties of inhomogeneous media. Appl. Phys. A **26**, 207–220 (1981)
12. Milton, G.W.: Bounds on the complex permittivity of a two- component composite material. J. Appl. Phys. **52**, 5286–5293 (1981)
13. Milton, G.W.: Bounds on the transport and optical properties of a two-component composite material. J. Appl. Phys. **52**, 5294–5304 (1981)
14. Milton, G.W.: Bounds on the electromagnetic elastic, and other properties of two-components composites. Phys. Rev. Lett. **46**, 542–545 (1981)
15. Milton, G.W.: Multicomponent composites, electrical network and new types of continued fraction. Part I. Commun. Math. Phys. **111**, 281–327 (1987)

16. Milton, G.W.: Multicomponent composites, electrical network and new types of continued fraction. Part II. Commun. Math. Phys. **111**, 329–372 (1987)
17. Milton, G.W.: The Theory of Composite, Cambridge Monographs on Applied and Computational Mathematics. Cambridge University Press, Cambridge (2002)
18. Tokarzewski, S.: Multipoint continued fraction approach to the bounds on effective transport coefficients of two-phase media. IFTR Rep. **4**, 3–171 (2005)
19. Tokarzewski, S.: Inequalities for bounds on effective transport coefficients of two-phase media from power expansions at real points. ZAMP **61**, 773–780 (2010)
20. Tokarzewski, S., Telega, J.J., Pindor, M., Gilewicz, J.: Basic inequalities for multipoint Padé approximants to Stieltjes functions. Arch. Mech. **56**(2), 141–153 (2002)
21. Wiener, O.: The theorie des mischkörpers für das feld des stationären strömung. erste abhandlung die mittelswertsätze für kraft, polarisation und energie. Abhandlungen der Mathematisch-Physischen Klasse der Königlich Sächsischen Gesellschaft der Wissenschaften **32**, 509–604 (1912)
22. Zhang, D., Cherkasov, E.: Reconstruction of spectral function from effective permittivity of a composite material using rational function approximations. J. Comput. Phys. **228**(15), 5390–5409 (2009)

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