

Stanisław Tokarzewski

**MULTIPOINT CONTINUED
FRACTION APPROACH TO THE
BOUNDS ON EFFECTIVE
TRANSPORT COEFFICIENTS
OF TWO-PHASE MEDIA**

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Redaktor Naczelny:

doc. dr hab. Zbigniew Kotulski

Recenzenci:

prof. dr hab. Jacek Gilewicz

doc. dr hab. Kazimierz Piechór

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Summary

The prediction of macroscopic coefficients λ_e of composites, if properties λ_1 and λ_2 and microstructures Θ_1 and Θ_2 of their constituents are known, is one of the most important problems of mechanics of inhomogeneous media. Due to the difficulty of calculating λ_e exactly, there has been much of interest in obtaining bounds on λ_e .

The main objective of this contribution is to establish in a coherent and unified form new S - and T - Multipoint Continued Fraction Methods (SMCFM and TMC FM) of an estimation of effective transport coefficients $\lambda_e(z)/\lambda_1$ of two-phase media for the cases, where the truncated power expansions of $\lambda_e(z)/\lambda_1$, $z = (\lambda_2/\lambda_1) - 1$ at a number of real points (SMCFM) and infinity (TMC FM) are known.

The SMC FM and TMC FM established in this work are the first methods of the theory of inhomogeneous media that incorporate into the bounds on $\lambda_e(z)/\lambda_1$ unlimited numbers of terms of the power series $(\lambda_e(z)/\lambda_1)$ expanded at several real points (SMCFM) and infinity (TMC FM). Especially the incorporation of the power expansion of $(\lambda_e(z)/\lambda_1)$ at infinity into the complex estimates of $(\lambda_e(z)/\lambda_1)$ is a very interesting and practically useful result, cf. [27, 58, 59, 44]. The SMC FM and TMC FM bounds on $(\lambda_e(z)/\lambda_1)$ are optimal over the given coefficients of the truncated power series $\lambda_e(z)/\lambda_1$.

Many nontrivial examples of applications of SMC FM and TMC FM are provided in the present work (cf. Section 4.3) and also in our earlier papers dealing with natural and man-made two-phase media. In the articles [52, 69] the influence of marrow on a complex rigidity of a long human bone is investigated. The papers [61, 63] deal with the complex dielectric constants of regular lattices of spheres, while [3, 37, 58, 60, 62, 64, 66, 68] and [21, 22, 51, 56, 57] explore the multipoint Padé bounds on the real effective conductivities of linear and quasilinear regular composites. A special Padé approximant techniques for an investigation of a macroscopic behavior of two-phase media are presented in [1, 2, 4, 5].

Wiener [73] gave optimal bounds on the effective coefficients of a multicomponent materials with fixed volume fractions of inclusions and real component parameters. Hashin and Shtrikman [30] improved Wiener's bounds using variational principles. Bergman [11, 13] introduced a method for obtaining bounds on complex effective parameters which does not rely on variational principles. Instead it exploited the properties of the effective parameters as analytic functions of the component parameters. The method of Bergman has been elaborated upon in detail and applied to several problems by Milton [41, 43], see also Felderhof [20].

A mathematical formulation for the Bergman's method was given by Golden and Papanicolaou [29]. The special continued fraction techniques for an investigation of a macroscopic behavior of two-phase media have been proposed by Bergman [14], Clark and Milton [17], Tokarzewski [53, 55] and Tokarzewski *et al.* [58, 67].

The SMC FM and TMC FM established here reduce in particular cases to the earlier continued fraction methods developed by Bergman [14], Clark and Milton [17], Tokarzewski [54, 55], Tokarzewski and Telega [66, 67], Gilewicz *et al.* [27], Tokarzewski *et al.* [71, 72] and Milton [44].

It is commonly known [44, Chap.18, pp.422] that on the trajectories depending on one parameter the eigenvalues of the effective coefficients of linear composites have Stieltjes integral representations with a positive-semidefinite Stieltjes measures, cf. (1.51). Hence the SMC FM and TMC FM established in this work can also be applied to any linear inhomogeneous materials, for example to viscous suspensions, porous materials, elastic and viscoelastic composites and also to media conducting heat and electrical current. How to do it in practise, it is a goal of our future work.

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AIMS AND SCOPE OF HABILITATION THESIS

Composites are prevalent in both nature and amongst engineered materials. Common metals, reinforced concretes, fiber glasses, colloidal suspensions, ceramics, bones et cetera are examples of natural and man-made composite media. Hence, the prediction of a macroscopic behavior of composites, if properties and microstructures of their constituents are known, is one of the most important problems of classical physics. There are three reasons of the study of composite materials distinguished by Milton in his excellent monograph [44].

The first one is to understand and then design nontrivial mechanical responses of inhomogeneous media to external forces acting on them. For example, suppose one is given two isotropic conducting materials: a metal with high conductivity, and a plastic which is electrically insulating. If one places these two materials in alternating layers in a laminate one obtains a highly anisotropic composite, which has the conducting properties of the metal in directions parallel to the layers and the insulating properties of the plastic normal to the layers. Concrete is cheap and relatively light, but breaks apart easily under tension. By contrast, steel is strong but expensive and heavy. By pouring the concrete around prestressed metal bars one obtains a composite, namely reinforced concrete, which is cheap, relatively light, and strong. Wood is an example of a material which is strong in the fiber direction but the fibers pull apart easily. By alternating layers of wood which are strong in the x_1 direction with layers of wood which are strong in the x_2 direction one obtains a plywood which is strong in two directions, i. e. (x_1, x_2) plane.

A second equally important reason is that what we learn from the field of composites could have far reaching implications in many fields of science. Significant progress in improving our understanding of how microscopic behavior influences macroscopic behavior could impact our understanding of turbulence, of phase transitions involving many length scales, of how quantum behavior influences behavior on classical length scales, or at more extreme level of how behavior on the Planck length scale, 10^{-33} cm, influences behavior on the atomic scale, 10^{-8} cm. While that may seem unlikely, its hard to deny the impact our understanding of classical physics had on the development of quantum mechanics. Therefore its conceivable that a better understanding of classical questions involving multiple length scales could have large reverberations.

A third compelling reason for studying composites is simply that there are many beautiful mathematical questions waiting for answers. The solution of some questions has already led to the development of new mathematical tools, and one can expect that the solution of the more challenging outstanding questions will open new mathematical frontiers.

The study of composites is a subject with a long history, which has attracted the interest of some of the greatest scientists. For example, Poisson [47] constructed a theory of induced magnetism, in which the body was assumed to be composed of conducting spheres embedded in a non-conducting material. Faraday [19] proposed a model for dielectric materials, consisting of metallic globules separated by insulating material. Maxwell [36] solved for the conductivity of a dilute suspension of conducting spheres in a conducting matrix. Rayleigh [48] found a system of linear equations, which when solved would give the effective conductivity of non-dilute square arrays of cylinders or cubic lattices of spheres. Einstein [18] calculated the effective shear viscosity of a suspension of rigid spheres in a fluid. The main historical developments of investigations of the composite materials are summarized in the articles [33] and [35].

Very efficient numerical algorithms are currently available for calculating the effective tensors of quite complicated two-dimensional microgeometries. The numerical evaluation

of the effective tensors for three-dimensional microgeometries is also progressing rapidly. In light of these advances one might ask: Why is there a need for developing bounds on effective tensors. One reason is that they often provide quick and simple estimates of the effective tensors.

Another reason for favoring bounds is that in most experiment situations we do not have a complete knowledge of the composite geometry. Even when an accurate determination of the three-dimensional composite microgeometry is possible, obtaining this information and numerically parameterizing it can be a very time-consuming process.

Bounds are also important in problems of structural optimization, where one needs to characterize the set of possible macroscopic responses of a composite as local properties vary over the set of admissible tensor fields, and to identify such fields that produce extreme responses.

It has been proved by Milton [44, Chap.18, Sec.18.6] that on trajectories depending on one parameter the eigenvalues of the effective coefficients of multicomponent materials have Stieltjes integral representations. Hence an evaluation of the bounds on the effective constants of linear and quasilinear composites reduces to a computation of the estimates of an effective transport coefficient of a two-phase medium or more precisely to a computation of the bounds on a Stieltjes function from its truncated power series.

In the theory of inhomogeneous media there are two continued fraction methods of an estimation of the effective transport coefficients of two-phase composite materials proposed by Bergman [14] (J -transformation method) and by Milton [44] (Y -transformation method). The methods mentioned can incorporate into the bounds on $\lambda_e(z)/\lambda_1$ the values $\lambda_e(x_j)/\lambda_1$, $j = 1, 2, \dots, N$, $x_j \in \mathbb{R}$ and several terms of the power series $\lambda_e(z)/\lambda_1$ constructed at $z = 0$.

In this work by starting from the mathematical results reported in [6, 9] we developed new S -transformation method of an estimation of the effective transport coefficients that deals with unlimited numbers of coefficients of the power expansions of $\lambda_e(z)/\lambda_1$ at N real points. We called it the S -Multipoint Continued Fraction Method (SMCFM) of an estimation of $\lambda_e(z)/\lambda_1$. However, the SMCFM derived by us possesses a significant disadvantage. It does not incorporate into the bounds on $\lambda_e(z)/\lambda_1$ the power series $\lambda_e(z)/\lambda_1$ expanded at infinity.

The main objective of this work is to overcome this disadvantage by establishing in a coherent and unified form new T -transformation method of an estimation of effective transport coefficients $\lambda_e(z)/\lambda_1$ of two-phase media called the T -Multipoint Continued Fraction Method (TMCFM). If the power expansion of $\lambda_e(z)/\lambda_1$ at infinity is not known the TMCFM reduces first to the SMCFM and next to J -, Y - transformation methods reported in literature, cf. [14] and [44].

The remainder of this work is organized as follows. In Chapter 1 the problem of effective coefficients of two-phase media leading to a Stieltjes integral is explored. In Chapters 2 the S - Multipoint Continued Fraction Method of an estimation of a Stieltjes function $f_1(z)$ from the truncated power series is derived. In Chapter 3 we establish the T -Multipoint Continued Fraction Method valid for the incomplete series expanded at both real points and infinity. In Chapter 4 the TMCFM is adapted to evaluate the T -continued fraction bounds on the effective constants $\lambda_e(z)/\lambda_1$ of two-phase composite. Many numerical examples computing T -bounds are provided. The list of conclusions together with the final remarks finish this work.

Chapter 1

PREDICTION OF EFFECTIVE TRANSPORT COEFFICIENTS IN TERMS OF STIELTJES FUNCTIONS

In this chapter the macroscopic thermal behavior of a composite consisting of two isotropic components is investigated. We prove that the nondimensional effective conductivity $(\lambda(z) - 1)/z$, $\lambda(z) = \lambda_e(z)/\lambda_1$, $z = (\lambda_2/\lambda_1) - 1$ has an anisotropic Stieltjes integral representation with a positive-semidefinite Stieltjes measure. Here λ_e and λ_1 , λ_2 denote the effective coefficient of a composite and the material constants of its constituents. The method of proving used by us differs from the procedures presented by Bergman [11], Golden Papanicolaou [29] and Milton [44, pp. 376].

The rigorous definition of a Stieltjes function $f_1(z)$ is introduced and compared with the corresponding one reported by Baker and Graves-Morris [9, Chap. 5]. We also explore the mathematical properties of Stieltjes functions $f_1(z)$ and $f_2(z)$ interrelated by S and T linear fractional transformations.

The results of this chapter are applied in the next ones to develop S - and T -Multipoint Continued Fraction Methods of an estimation of a Stieltjes function $f_1(z) = (\lambda(z) - 1)/z$ expanded at a number of real points and infinity.

1.1 Thermal conductivity coefficient by the homogenization procedure

We consider an infinite anisotropic medium. Let $u(X)$, $f(X)$, and $a_{ij}(X)$ denote the temperature field, the internal heat source density and the conductivity tensor, respectively, at a spatial point $X \in \mathbb{R}^3$. The temperature distribution $u(X)$ is then governed by the linear conductivity equation

$$-\frac{\partial}{\partial X_i} \left(a_{ij}(X) \frac{\partial u}{\partial X_j} \right) = f(X). \quad (1.1)$$

Now and in the sequel we assume that the phase geometry of a composite is periodic in the following sense:

$$a_{ij}(y + Y) = a_{ij}(y) \quad \forall y. \quad (1.2)$$

Relations (1.2) means that

- (i) We have subdivision of \mathbb{R}^3 in identical cells.
- (ii) The material is described by a Y -periodic conductivity tensor $a_{ij}(y)$, $y \in \mathbb{R}^3$, where Y -periodicity means that $a_{ij}(y_1) = a_{ij}(y_2)$ whenever y_1 and y_2 have the same position in the corresponding cells Y_1 and Y_2 . In particular we note that in a cell Y , Y -periodic functions take the same boundary values twice, but with opposite outer normal on the opposite faces of Y . Thus, for a Y -periodic vector field $f_i(y)$,

$$\int_Y \frac{\partial f_i(y)}{\partial y_i} dy = \int_{\partial Y} f_i(y) n_i dS = 0 \quad (1.3)$$

by Gauss theorem, where dS denotes two-dimensional area element of the unit cell walls ∂Y .

- (iii) We have scale factor $\varepsilon > 0$ such that the conductivity tensor for the body is defined as $a_{ij}^\varepsilon(X) = a_{ij}(X/\varepsilon)$. The variable $y = X/\varepsilon$ describing the Y -cell is called a local variable.

Let the parameter ε vary. Thereby we obtain a whole class of homothetically equivalent materials, where ε measures the fineness of the material. We also obtain a class of linear conductivity equations:

$$-\frac{\partial}{\partial X_i} \left(a_{ij} \left(\frac{X}{\varepsilon} \right) \frac{\partial u^\varepsilon(X)}{\partial X_j} \right) = f(X), \text{ Einstein summation convention.} \quad (1.4)$$

For our purposes the temperature distribution $u_0(X)$ defined by

$$u^\varepsilon(X)_{\varepsilon \rightarrow 0} = u_0(X) \quad (1.5)$$

is of interest only. Further on from the Eqs (1.4) and (1.5) it will be derived the equivalent equation

$$-\frac{\partial}{\partial X_i} \left(Q_{ik} \frac{\partial u_0(X)}{\partial X_k} \right) = f(X) \quad (1.6)$$

determining $u_0(X)$ called *the homogenized equation* for a linear composite materials (1.6). Here Q and $u_0(X)$ are *the effective conductivity coefficient* and *the homogenized temperature field*, respectively.

We assume that $u^\varepsilon(X)$ appearing in (1.4) can be represented by the asymptotic expansions of the form

$$u^\varepsilon(X) = w_0(X, y) + \varepsilon w_1(X, y) + \varepsilon^2 w_2(X, y) + \dots, \quad y = X/\varepsilon, \quad (1.7)$$

where the terms $w_j(X, y)$, $j = 0, 1, 2, \dots$ are Y -periodic. Now we define the operator A^ε by

$$A^\varepsilon \Psi = -\frac{\partial}{\partial X_i} \left(a_{ij}^\varepsilon(X) \frac{\partial \Psi}{\partial X_j} \right). \quad (1.8)$$

By setting $\Psi(X) = \Phi(X, y)$, $y = X/\varepsilon$ we can represent A^ε as

$$A^\varepsilon \Psi = (\varepsilon^{-2} A_0 + \varepsilon^{-1} A_1 + A_2) \Phi, \quad (1.9)$$

where

$$\begin{aligned} A_0 &= -\frac{\partial}{\partial y_i} \left(a_{ij}(y) \frac{\partial}{\partial y_j} \right), \\ A_1 &= -\frac{\partial}{\partial y_i} \left(a_{ij}(y) \frac{\partial}{\partial X_j} \right) - \frac{\partial}{\partial X_i} \left(a_{ij}(y) \frac{\partial}{\partial y_j} \right), \\ A_2 &= -\frac{\partial}{\partial X_i} \left(a_{ij}(y) \frac{\partial}{\partial X_j} \right), \text{ etc...} \end{aligned} \quad (1.10)$$

Eq. (1.4) can be rewritten as follows

$$(\varepsilon^{-2} A_0 + \varepsilon^{-1} A_1 + A_2) (w_0 + \varepsilon w_1 + \varepsilon^2 w_2 + \dots) = f. \quad (1.11)$$

By identifying the coefficients of the same powers of ε we obtain the following three lowest order equations

$$A_0 w_0 = 0, \quad (1.12)$$

$$A_0 w_1 + A_1 w_0 = 0, \quad (1.13)$$

$$\begin{aligned} A_0 w_2 + A_1 w_1 + A_2 w_0 &= f, \\ \dots\dots\dots, \text{ etc.} \end{aligned} \quad (1.14)$$

We can now use Eqs (1.12), (1.13) and Y -periodicity of w_0 to conclude, that w_0 does not depend on y . On account of that we have at once

$$w_0(X, y) = w_0(X) = u_0(X), \quad (1.15)$$

$$w_1(X, y) = -\chi^k(y) \frac{\partial u_0(X)}{\partial X_k} + u_1(X), \quad (1.16)$$

where $u_0(X)$ and $u_1(X)$ are arbitrary twice differentiable functions of X , while $\chi^j(y)$ is a solution of the cell problem

$$-A_0 \chi^k(y) = \frac{\partial}{\partial y_i} a_{ik}(y), \quad \chi^j(y) \quad Y - \text{periodic (see page 11)}. \quad (1.17)$$

Furthermore we conclude that (1.14) possesses a stationary Y -periodic solution if

$$\int_Y (f - A_1 w_1 - A_2 w_0) dy = 0. \quad (1.18)$$

By inserting the expressions (1.15) and (1.16) for w_0 and w_1 , respectively, into (1.18) we obtain

$$\begin{aligned} & \int_Y \left(f - \frac{\partial}{\partial y_i} (a_{ij} \chi^k) \frac{\partial^2 u_0(X)}{\partial X_i \partial X_k} + \frac{\partial a_{ij}}{\partial y_i} \frac{\partial u_1(X)}{\partial X_j} + \right. \\ & \left. - \frac{\partial}{\partial X_i} \left(a_{ij} \frac{\partial \chi^k}{\partial y_j} \frac{\partial u_0(X)}{\partial X_k} \right) + \frac{\partial}{\partial X_i} \left(a_{ik} \frac{\partial u_0(X)}{\partial X_k} \right) \right) dy = 0. \end{aligned} \quad (1.19)$$

The functions a_{ij} and χ^j are Y -periodic, while the functions $u_0(X)$ and $u_1(X)$ are independent of y . Therefore the second and the third terms of the integral (1.19) vanish by the Gauss theorem and Eq.(1.19) simplifies to Eq. (1.6), where components Q_{ik} are equal to

$$Q_{ik} = \frac{1}{|Y|} \int_Y \left(a_{ik}(y) - a_{ij}(y) \frac{\partial \chi^{(k)}(y)}{\partial y_j} \right) dy, \quad (1.20)$$

while the auxiliary functions $\chi^k(y)$ satisfy (1.17)

$$\frac{\partial}{\partial y_i} \left(a_{ij}(y) \frac{\partial \chi^{(k)}(y)}{\partial y_j} \right) = \frac{\partial}{\partial y_i} a_{ik}(y), \quad \chi^{(k)}(y) \quad Y - \text{periodic}. \quad (1.21)$$

By substituting $\chi^{(k)}(y) = y_k - T^k$ into (1.20) and (1.21) we obtain

$$Q_{ik} = \frac{1}{|Y|} \int_Y a_{ij}(y) \frac{\partial T^{(k)}(y)}{\partial y_j} dy, \quad (1.22)$$

$$-\frac{\partial}{\partial y_i} a_{ij}(y) \frac{\partial T^{(k)}(y)}{\partial y_j} = 0, \quad (y_k - T^{(k)}) \quad Y - \text{periodic}. \quad (1.23)$$

For isotropic case ($a_{ij} = a \delta_{ij}$) the relations (1.22) and (1.23) reduce to

$$Q_{ik} = \frac{1}{|Y|} \int_Y a(y) \frac{\partial T^{(k)}(y)}{\partial y_i} dy, \quad (1.24)$$

$$-\frac{\partial}{\partial y_i} \left(a(y) \frac{\partial T^{(k)}(y)}{\partial y_i} \right) = 0, \quad (y_k - T^{(k)}) \quad Y - \text{periodic}. \quad (1.25)$$

In the sequel we consider the two-phase material only with a thermal conductivity coefficient $a(y)$ given by

$$\frac{a(y)}{\lambda_1} = \Theta_1(y) + \frac{\lambda_2}{\lambda_1} \Theta_2(y) = 1 + z\Theta_2(y), \quad z = h - 1, \quad h = \frac{\lambda_2}{\lambda_1}, \quad (1.26)$$

where $\Theta_1(y)$ and $\Theta_2(y)$ are the characteristic functions of inclusions $\Theta_1(y) + \Theta_2(y) = 1$. By substituting (1.26) in (1.24)-(1.25) and taking into account the Eq. (1.6) one obtains a homogenized equation valid for macroscopically anisotropic two-phase medium (see also (1.6))

$$-\frac{\partial}{\partial X_j} Q_{jk}(z) \frac{\partial u_0(X)}{\partial X_j} = f(X), \quad (1.27a)$$

$$q_{jk}(z) = \frac{Q_{jk}(z)}{\lambda_1} = \frac{1}{|Y|} \int_Y (1 + z\Theta_2(y)) \frac{\partial T^{(j)}(y)}{\partial y_k} dy, \quad (1.28)$$

$$\frac{\partial}{\partial y_k} (1 + z\Theta_2(y)) \frac{\partial T^{(j)}(y)}{\partial y_k} = 0, \quad (y_j - T^{(j)}) \text{ } Y\text{-periodic.} \quad (1.29)$$

Note that $Q_{ij}(z)$ does not depend on the spatial variable X . In the next chapter we will prove that the diagonals of the homogenized coefficient $(q_{jk}(z) - \delta_{jk})/z$ resulting from (1.28) and (1.29) have a Stieltjes integral representation.

1.2 Stieltjes integral representation for a homogenized thermal conductivity

On the basis of the Y -periodicity of the functions $(y_k - T^{(k)})$ the Eqs (1.28) and (1.29) can be rewritten as follows

$$\frac{q_{jk}(z) - \delta_{jk}}{z} = \frac{1}{|Y|} \int_Y \Theta_2(y) \frac{\partial T^{(j)}(y)}{\partial y_k} dy, \quad (1.30)$$

$$\frac{\partial}{\partial y_k} \frac{\partial T^{(j)}(y)}{\partial y_k} = -z \frac{\partial}{\partial y_k} \Theta_2(y) \frac{\partial T^{(j)}(y)}{\partial y_k}, \quad (y_j - T^{(j)}) \text{ } Y\text{-periodic.} \quad (1.31)$$

With the help of a periodic Green function $G(y, y')$

$$\frac{\partial}{\partial y_i} \frac{\partial}{\partial y_i} G(y, y') = - \left(\delta^3(y - y') - \frac{1}{|Y|} \right), \quad G(y, y') \text{ } Y\text{-periodic} \quad (1.32)$$

the boundary value problem (1.31) can now be recast as an integral equation

$$T^{(k)} = y_k - z\Gamma T^{(k)} \quad (1.33)$$

equivalent to (1.31). Here

$$\Gamma T^{(k)} \equiv \int_{Y'} \Theta_2(y') \frac{\partial}{\partial y'_i} G(y, y') \frac{\partial}{\partial y'_i} T^{(k)}(y') dy' \quad (1.34)$$

is a linear operator mapping the continuous functions $T^{(k)}(y')$ defined in Y' into the Y -periodic ones defined in Y . This operator is selfadjont, if the scalar product of potentials $\alpha(y)$ and $\beta(y)$ is defined by

$$\langle \alpha, \beta \rangle = \int_Y \Theta_2(y) \frac{\partial}{\partial y_i} \alpha(y) \frac{\partial}{\partial y_i} \beta(y) dy. \quad (1.35)$$

Hence the equation (1.30) takes the form

$$\frac{q_{jk}(z) - \delta_{jk}}{z} = \frac{1}{|Y|} \langle y_j, T^{(k)} \rangle = \frac{1}{|Y|} \langle y_j, (1 + z\Gamma)^{-1} y_k \rangle. \quad (1.36)$$

Here we substituted the solution of (1.33), i.e. $T^{(k)} = (1 + z\Gamma)^{-1} y_k$. Since Γ is selfadjont, it has a complete set of eigenfunctions ϕ_n with real eigenvalues U_n

$$\Gamma \phi_n = U_n \phi_n. \quad (1.37)$$

Let us introduce a periodic function

$$f_j(y) = \sum_n \langle y_j, \phi_n(y) \rangle \phi_n(y), \quad n = 1, 2, \dots \quad (1.38)$$

From (1.38), it follows that

$$\langle f_j(y), \phi_k(y) \rangle = \langle y_j, \phi_k(y) \rangle. \quad (1.39)$$

Relations (1.34) and (1.39) yield immediately

$$f_j(y) = y_j \text{ for } y \text{ satisfying } \Theta_2(y) = 1. \quad (1.40)$$

Since the characteristic functions $\Theta_2(y)$ appear in (1.35) the following identities hold

$$\langle y_j, f_k \rangle = \langle y_j, y_k \rangle, \quad \Gamma f_k = \Gamma y_k \quad (1.41)$$

and on account of (1.36) we have

$$\frac{q_{jk}(z) - \delta_{jk}}{z} = \frac{1}{|Y|} \langle y_j, (1 + z\Gamma)^{-1} y_k \rangle = \frac{1}{|Y|} \langle y_j, (1 + z\Gamma)^{-1} f_k \rangle. \quad (1.42)$$

Let us expand $(1 + z\Gamma)^{-1}$ in the formal power series

$$(1 + z\Gamma)^{-1} = \sum_{m=0}^{\infty} (-z\Gamma)^m. \quad (1.43)$$

By (1.43) to (1.38) one obtains

$$(1 + z\Gamma)^{-1} f_k = \sum_{m=0}^{\infty} (-z\Gamma)^m f_k = \sum_n \frac{\langle y_k, \phi_n \rangle \phi_n}{1 + zU_n}. \quad (1.44)$$

Due to (1.44) the relation (1.36) takes the form

$$\frac{q_{jk}(z) - \delta_{jk}}{z} = \sum_n \frac{\Lambda_{jk}^{(n)}}{1 + zU_n}, \quad (1.45)$$

where the symmetrical tensor $\Lambda_{jk}^{(n)}$ is equal to

$$\Lambda_{jk}^{(n)} = \langle y_j, \phi_n \rangle \langle y_k, \phi_n \rangle. \quad (1.46)$$

The eigenvalues of $\Lambda^{(n)}(U_n)$ given by (1.46) are non-negative. Hence $\Lambda^{(n)}(U_n)$ is a positive semi-definite tensor

$$\Lambda^{(n)}(U_n) \geq 0. \quad (1.47)$$

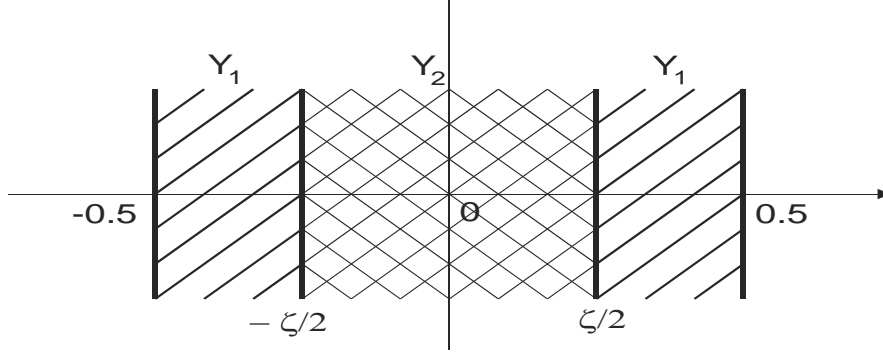


Fig. 1.1 The unit cell of a periodic, one-dimensional two-phase material occupying the regions Y_1 and Y_2 , ξ -volume fraction.

For physical realistic values of $z \in (-1, \infty)$ the diagonal components of an effective tensor (1.45) take finite values only (cf. [14])

$$\frac{q_{ii}(z) - 1}{z} = \sum_n \frac{\Lambda_{ii}^{(n)}}{1 + zU_n} < \infty \text{ for } -1 < z < \infty, \quad i = 1, 2, 3. \quad (1.48)$$

On account of that the positions of the poles z_n of $\frac{q_{ii}(z)-1}{z}$, if they are, satisfy the relation ((cf. (1.48))

$$-\infty \leq z_n \leq -1. \quad (1.49)$$

The inequality (1.49) applied to (1.48) yields at once the range of admissible values of U_n .

$$0 \leq U_n \leq 1. \quad (1.50)$$

Now it is convenient to rewrite (1.45), (1.47) and (1.50) as follows

$$\frac{q_{jk}(z) - \delta_{jk}}{z} = \int_0^1 \frac{d\gamma_{jk}(u)}{1 + zu}, \quad d\gamma_{jk}(u) \geq 0, \quad (1.51)$$

where

$$\gamma_{jk}(u) = \sum_n \Lambda_{jk}^{(n)}(U_n) H(u - U_n), \quad n = 1, 2, \dots, \quad H(u) = \begin{cases} 0 & \text{if } u < 0, \\ 1 & \text{if } u \geq 0. \end{cases} \quad (1.52)$$

The Stieltjes integral representation of the effective coefficients given by (1.51)-(1.52) was derived by Bergman [11], next by Golden and Papanicolaou [29] and very recently by Milton [44, pp. 376, Eq. 18.15]. The derivation procedures used by them differ from that one presented in this section.

1.3 One dimensional composite material.

In order to illustrate the results of Section 1.2 we will investigate the periodic composite consisting of two-phase unit cells depicted in Fig.1.1. Under the assumption $|Y| = 1$ the Eqs (1.30)-(1.31) reduce to

$$\frac{\lambda(z) - 1}{z} = \int_Y \Theta_2(y) \frac{\partial T(y)}{\partial y} dy, \quad (1.53)$$

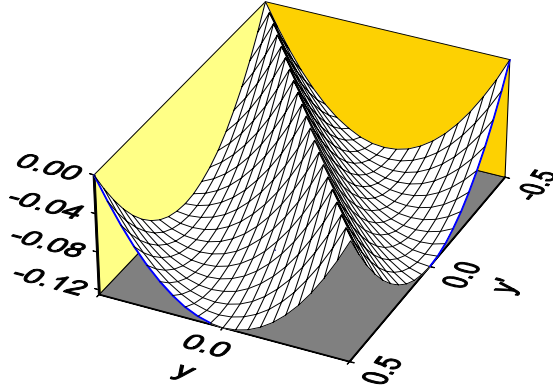


Fig. 1.2 Periodic Green function $G(y, y')$ for the one-dimensional Laplace equation, cf. (1.55).

$$\frac{\partial^2 T(y)}{\partial y^2} = -z \frac{\partial}{\partial y} \Theta_2(y) \frac{\partial T(y)}{\partial y}, \quad (y - T) \text{ Y-periodic}, \quad (1.54)$$

while the relation (1.32) to

$$\frac{\partial^2 G(y, y')}{\partial y^2} = -(\delta(y - y') - 1), \quad G(y, y') \text{ Y-periodic}. \quad (1.55)$$

The solution of (1.55) is given by

$$G(y, y') = \frac{1}{2}(y - y')^2 - \frac{1}{2}|y - y'|. \quad (1.56)$$

The periodic one-dimensional Green function (1.56) is shown in Fig. 1.2. A complete set of U_n, ϕ_n satisfying (1.37)

$$\int_{-\zeta/2}^{\zeta/2} \frac{\partial}{\partial y'} G(y, y') \frac{\partial}{\partial y'} \phi_1(y') dy' = U_1 \phi_1(y) \quad (1.57)$$

and (cf. (1.38)-(1.41))

$$\langle y, f \rangle = \langle y, \phi_1(y) \rangle \langle y, \phi_1(y) \rangle = \langle y, y \rangle \quad (1.58)$$

reduces to the one positive eigenvalue U_1 associated with the eigenfunction ϕ_1

$$U_1 = (1 - \zeta), \quad \phi_1(y) = \begin{cases} \frac{\sqrt{\zeta}}{1 - \zeta}(-y - 1/2) & \text{for } y \in (-1/2, -\zeta/2), \\ \sqrt{\frac{1}{\zeta}}y & \text{for } y \in (-\zeta/2, \zeta/2), \\ \frac{\sqrt{\zeta}}{1 - \zeta}(-y + 1/2) & \text{for } y \in (\zeta/2, 1/2). \end{cases} \quad (1.59)$$

Here ζ denotes the volume fraction of inclusions, see Fig. 1.1. Due to (1.28), (1.45) and (1.59) the effective transport coefficient $(\lambda - 1)/z$ of a periodic one-dimensional composite is given by

$$\frac{\lambda - 1}{z} = \frac{\langle y, \phi_1 \rangle \langle y, \phi_1 \rangle}{1 + zU_1} = \frac{\zeta}{1 + (1 - \zeta)z}. \quad (1.60)$$

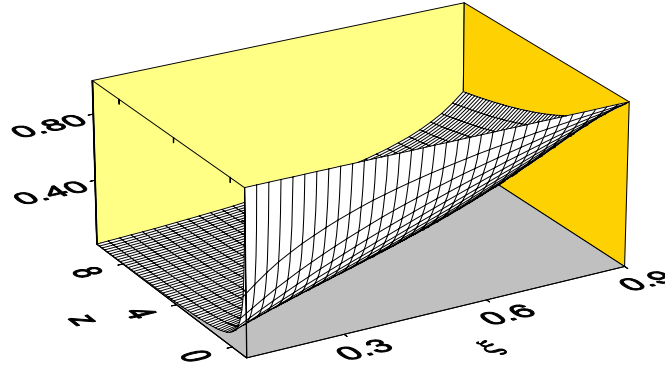


Fig. 1.3 The effective transport coefficients $(\lambda - 1)/z$ of a periodic one-dimensional two-phase medium, cf. (1.60).

The coefficient $(\lambda - 1)/z$ is shown in Fig. 1.3 versus z and ζ . Note that for a fixed ζ the modulus $(\lambda - 1)/z$ (1.60) has a Stieltjes integral representation

$$\frac{\lambda - 1}{z} = \int_0^1 \frac{d\beta(u)}{1 + zu}, \quad \beta(u) = \zeta H(u - (1 - \zeta)). \quad (1.61)$$

By substituting $z = \lambda_2/\lambda_1 - 1$ and $\lambda(z) = \lambda_e/\lambda_1$ into (1.60) one arrives at

$$\lambda_e = 1 + z \frac{\zeta}{1 + z(1 - \zeta)} = \frac{1}{\frac{1 - \zeta}{\lambda_1} + \frac{\zeta}{\lambda_2}}. \quad (1.62)$$

Formula (1.62) obtained by means of a homogenization procedure (see (1.53)-(1.54)) coincides with the classical lower bound on λ_e established by Wiener via the variational method, cf. [73].

1.4 Effective transport coefficients of two-phase media represented by Stieltjes functions

Now our investigations will be limited to the composite materials possessing the isotropic symmetry only (cf.(1.51))

$$q_{11} = q_{22} = q_{33} = \lambda, \quad q_{12} = q_{23} = q_{13} = 0. \quad (1.63)$$

For such a case the anisotropic transport coefficient (1.51) reduces to (cf. (1.63))

$$f_1(z) = \frac{\lambda(z) - 1}{z} = \int_0^1 \frac{d\gamma_1(u)}{1 + zu}, \quad d\gamma_1(u) \geq 0. \quad (1.64)$$

For further purposes the mathematical definition of a Stieltjes function is required:

Definition 1.1 *The Stieltjes integral*

$$f_1(z) = \int_0^{1/\rho} \frac{d\gamma_1(u)}{1 + zu}, \quad \rho \geq 0, \quad d\gamma_1(u) \geq 0 \quad (1.65)$$

we call the Stieltjes function, provided the real-valued moments μ_j of $\gamma_1(u)$

$$\mu_j = \int_0^{1/\rho} u^j d\gamma_1(u), \quad j = 0, 1, 2, \dots \quad (1.66)$$

are finite

According to (1.65).and (1.66) the effective transport coefficient $(\lambda - 1)/z$ given by (1.64) is a Stieltjes function.

Now we start discussing of the basic properties of the Stieltjes function $f_1(z)$, cf. Definition 1.1. From (1.65), it follows that $f_1(z)$ is a *real symmetric* function, defined in the complex z -plane with the cut $[-\infty, -\rho]$ on the negative real axis. A function $f_1(z)$ is *real symmetric*, if it satisfies the relation $f_1(z^*) = [f_1(z)]^*$, where z^* denotes the complex conjugate of z .

The power series expansion of $f_1(z)$ at $z = 0$ is called the series of Stieltjes (cf. (1.65), (1.66))

$$f_1(z) = \sum_{j=0}^{\infty} c_j(0)z^j, \quad c_j(0) = \frac{f_1^{(j)}(0)}{j!} \equiv (-1)^j \mu_j. \quad (1.67a)$$

It is convergent on the complex plane in the disk

$$|z| < \rho, \quad \rho > 0. \quad (1.68)$$

Moreover, from (1.65) follows that the power expansions

$$f_1(z) = \sum_{j=0}^{\infty} c_j(x_k)(z - x_k)^j, \quad c_j(x_k) = \frac{f_1^{(j)}(x_k)}{j!}, \quad k = 1, 2, \dots, N \quad (1.69)$$

are convergent in the disks

$$|z - x_k| < \rho + x_k, \quad k = 1, 2, \dots, N. \quad (1.70)$$

The coefficients $c_j(x_k)$, $j = 0, 1, 2, \dots$ are real if and only if $f_1(z)$ is real symmetric. In many practical situations it is convenient to approximate the Stieltjes functions $f_1(z)$ by the sums of simple fractions of the type $\frac{C_{n,J}}{1+zU_{n,J}}$. To this end we formulate the following lemma:

Lemma 1.2 For $n = 0, 1, 2, \dots, J$ and

$$0 < C_{n,J} < \infty, \quad 0 \leq U_{0,J} < U_{1,J} < \dots < U_{J,J} \leq \infty, \quad J = 1, 2, \dots \quad (1.71)$$

the relations

$$f_1(z) = \int_0^{\infty} \frac{d\gamma_1(u)}{1+zu} = \sum_{n=0}^J \frac{C_{n,J}}{1+zU_{n,J}}, \quad d\gamma_1(u) > 0, \quad J \rightarrow \infty \quad (1.72)$$

are satisfied, provided that

$$\gamma_1(U_{n,J}) - \gamma_1(U_{n-1,J}) = C_{n,J}. \quad (1.73)$$

Proof. From (1.71₂), it follows that

$$\max \{(U_{n,J} - U_{n-1,J}); \quad n = 0, 1, 2, \dots, J\} \rightarrow 0 \text{ if } J \rightarrow \infty. \quad (1.74)$$

Due to the relations (1.74) and Eqs [49, Eqs 1 and 2, pp. 97] the relation (1.72) is satisfied. ■

In the next section the Lemma (1.2) will be used to investigate the properties of the Stieltjes functions interrelated by S - and T - linear fractional transformations.

1.5 Linear fractional transformation of Stieltjes functions

In this section the properties of Stieltjes functions interrelated by linear fractional transformations of type S

$$f_1(z) = \frac{f_1(a)}{1 + (z - a)f_2(z)}, \quad a \in \mathbb{R}, \quad z \in \mathbb{C} \quad (1.75)$$

and type T

$$f_1(z) = \frac{f_1(a)}{1 + (z - a)\frac{f_1(a)}{\varphi_1(\infty)} + (z - a)f_2(z)}, \quad \varphi_1(\infty) = \lim_{z \rightarrow \infty} z f_1(z), \quad z \in \mathbb{C} \quad (1.76)$$

are investigated.

Lemma 1.3 *For z satisfying the inequality*

$$\begin{aligned} |1 + (z - a)f_2(z)| > 0, \quad z \neq a \in \mathbb{R}, \quad z \in \mathbb{C} \\ \left(\left| 1 + (z - a)\frac{f_1(a)}{\varphi_1(\infty)} + (z - a)f_2(z) \right| > 0, \quad \varphi_1(\infty) = \lim_{z \rightarrow \infty} z f_1(z) \right) \end{aligned} \quad (1.77)$$

the S -linear fractional transformation (T -linear fractional transformations) of $f_2(z)$ to $f_1(z)$ and inversely of $f_1(z)$ to $f_2(z)$ are continuous operations, cf. (1.75)-(1.76).

Proof. Consider the Stieltjes functions $f_1(z)$, $f''_1(z)$ and $f_2(z)$, $f''_2(z)$ interrelating by (1.75)

$$f_1(z) = \frac{f_1(a)}{1 + (z - a)f_2(z)}, \quad f''_1(z) = \frac{f''_1(a)}{1 + (z - a)f''_2(z)}. \quad (1.78)$$

From (1.78), it follows

$$f_1(z) - f''_1(z) = \frac{f_1(a) - f''_1(a) + (z - a)(f_1(a)f''_2(z) - f''_1(a)f_2(z))}{(1 + (z - a)f_2(z))(1 + (z - a)f''_2(z))}. \quad (1.79)$$

Hence for $f''_1(z) \rightarrow f_1(z)$ we have

$$\lim_{f''_1(z) \rightarrow f_1(z)} f_1(z) - f''_1(z) = \lim_{f''_1(z) \rightarrow f_1(z)} \frac{(z - a)f_1(a)(f''_2(z) - f_2(z))}{(1 + (z - a)f_2(z))(1 + (z - a)f''_2(z))}, \quad (1.80)$$

while for $f''_2(z) \rightarrow f_2(z)$ one obtains

$$\lim_{f''_2(z) \rightarrow f_2(z)} f_1(z) - f''_1(z) = \lim_{f''_2(z) \rightarrow f_2(z)} \frac{(z - a)f_1(a)(f''_2(z) - f_2(z))}{(1 + (z - a)f_2(z))^2}. \quad (1.81)$$

For z satisfying (1.77₁) and $z \neq a$ the relations (1.79) and (1.80) yield at once

$$\text{if } \lim_{|f_1(z) - f''_1(z)| \rightarrow 0} = 0 \quad \text{then} \quad \lim_{|f_2(z) - f''_2(z)| \rightarrow 0} = 0. \quad (1.82)$$

and

$$\text{if } \lim_{|f_2(z) - f''_2(z)| \rightarrow 0} = 0 \quad \text{then} \quad \lim_{|f_1(z) - f''_1(z)| \rightarrow 0} = 0. \quad (1.83)$$

Thus for the case of S -transformation the proof is complete. For T -transformation it will be proceeded analogously. ■

Lemma 1.3 jointly with Lemma 1.2 allow us to represent Stieltjes functions $f_1(z)$ and $f_2(z)$ as a sums of simple fractions and next interrelate those sums by the linear fractional transformations of type S and T , see (1.75) and (1.76).

1.5.1 Linear fractional transformation of $f_1(z)$ to $f_2(z)$

Let us consider two rational Stieltjes functions $f_{1,J}(z)$ and $f_{2,J}(z)$ given by

$$f_{1,J}(z) = \sum_{n=0}^J \frac{C_{n,J}^{(1)}}{1 + zU_{n,J}^{(1)}} \text{ in } z \in (-\infty, \infty),$$

$$0 < C_{n,J}^{(1)}, \quad n = 0, 1, 2, \dots, J,$$
(1.84)

$$U_{0,J}^{(1)} = 0 \quad (U_{0,J}^{(1)} > 0), \quad 0 < U_{n-1,J}^{(1)} < U_{n,J}^{(1)} \leq \infty, \quad n = 2, 3, \dots, J$$

and

$$f_{2,J}(z) = \sum_{n=0}^J \frac{C_{n,J}^{(2)}}{1 + zU_{n,J}^{(2)}} \text{ in } z \in (-\infty, \infty),$$

$$0 \leq C_{n,J}^{(2)}, \quad n = 1, 2, \dots, J,$$
(1.85)

$$U_{0,J}^{(2)} = \infty \quad (U_{0,J}^{(2)} = 0), \quad 0 < U_{n-1,J}^{(2)} < U_{n-1,J}^{(1)} < U_{n,J}^{(2)} < U_{n,J}^{(1)}, \quad n = 2, 3, \dots, J,$$

where J is a positive integer, while $C_{l,J}^{(k)}$ and $U_{l,J}^{(k)}$, $k = 1, 2$ are the real numbers. The notations $U_{0,J}^{(1)} = 0$ ($U_{0,J}^{(1)} = \infty$) and $U_{0,J}^{(2)} > 0$ ($U_{0,J}^{(2)} = 0$) appearing in (1.84) and (1.85) mean that

$$\text{if } U_{0,J}^{(1)} = 0 \text{ then } U_{0,J}^{(2)} = \infty \text{ and if } U_{0,J}^{(1)} > 0 \text{ then } U_{0,J}^{(2)} = 0.$$
(1.86)

We denote the real, negative roots of $f_{1,J}(z) = 0$ by $Z_{k,J}^{(1)}$

$$\sum_{n=0}^J \frac{C_{n,J}^{(1)}}{1 + Z_{k,J}^{(1)} C_{n,J}^{(1)}} = 0, \quad -\infty \leq Z_{0,J}^{(1)} < Z_{1,J}^{(1)} < \dots < Z_{J,J}^{(1)} < 0,$$
(1.87)

while the first derivatives of $f_{1,J}(z)$ at $Z_{k,J}^{(1)}$ by $f'_{1,J}(Z_{k,J}^{(1)})$

$$f'_{1,J}(Z_{k,J}^{(1)}) = - \sum_{n=0}^J \frac{C_{n,J}^{(1)} U_{n,J}^{(1)}}{\left(1 + Z_{k,J}^{(1)} U_{n,J}^{(2)}\right)^2} < 0, \quad k = 0, 1, \dots, J.$$
(1.88)

If the inequalities (1.84_{2,3}) are satisfied the negative roots $Z_{n,J}^{(1)}$, $k = 0, 1, \dots, J$ (1.87) and negative first derivatives $f'_{1,J}(Z_{k,J}^{(1)})$ (1.88) exist only.

Lemma 1.4 *If the functions (1.84) and (1.85) are interrelated by S -linear fractional transformation*

$$f_{1,J}(z) = \frac{f_{1,J}(a)}{1 + (z - a)f_{2,J}(z)}, \quad a \in \left(-\frac{1}{U_{J,J}^{(1)}}, \infty\right)$$
(1.89)

then $U_{n,J}^{(2)}$, $C_{n,J}^{(2)}$ depend on $C_{n,J}^{(1)}$, $U_{n,J}^{(1)}$ as follows

$$U_{n,J}^{(2)} = -\frac{1}{Z_{n,J}^{(1)}}, \quad C_{n,J}^{(2)} = \frac{f_{1,J}(a)U_{n,J}^{(2)}}{f'_{1,J}(Z_{n,J}^{(1)})(Z_{n,J}^{(1)} - a)}, \quad n = 1, 2, \dots, J.$$
(1.90)

Moreover, the inequalities (1.85_{2,3}) are immediate consequence of the relations (1.90) and (1.84_{2,3}).

Proof. By substituting (1.84)-(1.85) into (1.89) one obtains

$$f_{1,J}^l(z) = f_{1,J}^r(z), \quad (1.91)$$

where

$$f_{1,J}^l(z) = C_{0,J}^{(1)} + \sum_{n=1}^J \frac{C_{n,J}^{(1)}}{1 + zU_{n,J}^{(1)}}, \quad f_{1,J}^r(z) = \frac{f_{1,2}(a)}{1 + (z-a) \left(\sum_{n=1}^J \frac{C_{n,J}^{(2)}}{1 + zU_{n,J}^{(2)}} \right)}. \quad (1.92)$$

The equations

$$f_{1,J}^l(Z_{k,J}^{(1)}) = 0, \quad f_{1,J}^r(Z_{k,J}^{(1)}) = 0, \quad k = 1, 2, \dots, J, \quad (1.93)$$

$$\left. \frac{df_{1,J}^l(z)}{dz} \right|_{Z_{k,J}^{(1)}} = \left. \frac{df_{1,J}^r(z)}{dz} \right|_{Z_{k,J}^{(1)}}, \quad k = 1, 2, \dots, J$$

yield the relations (1.90) at once. The inequalities (1.85_{2,3}) are consequence of (1.84_{2,3}) and (1.87)-(1.88). The proof is complete. ■

Example 1.5 Consider the rational function

$$f_{1,3}(z) = \frac{0.1667}{1 + 0.3334z} + \frac{0.25}{1 + 0.5z} + \frac{0.3334}{1 + 0.75z} + \frac{0.5}{1 + z}, \quad (1.94)$$

$$a = 1, \quad U_{0,3}^{(1)} > 0, \quad f_{1,3}(1) = 0.7321.$$

From (1.87), (1.90) and (1.94), it follows

$$Z_{0,3}^{(1)} = -\infty, \quad Z_{1,3}^{(1)} = -2.6467, \quad Z_{2,3}^{(1)} = -1.6876, \quad Z_{3,3}^{(1)} = -1.1514, \quad (1.95)$$

$$U_{0,3}^{(2)} = \lim_{z_1^{(1)} \rightarrow -\infty} \frac{1}{Z_{0,3}^{(1)}} = 0, \quad U_{1,3}^{(2)} = 0.3778, \quad U_{2,3}^{(2)} = 0.5925, \quad U_{3,3}^{(2)} = 0.8685, \quad (1.96)$$

$$C_{0,3}^{(2)} = 0.3765, \quad C_{1,3}^{(2)} = 0.0134, \quad C_{2,3}^{(2)} = 0.0161, \quad C_{3,3}^{(2)} = 0.0082. \quad (1.97)$$

By substituting (1.95)-(1.97) into (1.85) one obtains

$$f_{2,3}(z) = \frac{0.3765}{1} + \frac{0.0134}{1 + 0.3778z} + \frac{0.0161}{1 + 0.5925z} + \frac{0.0082}{1 + 0.8685z}. \quad (1.98)$$

The inequalities (1.84_{2,3}) and (1.85_{2,3}) are satisfied, cf. (1.94) and (1.98).

Now on the basis of Lemma 1.4 we can state:

Lemma 1.6 If the Stieltjes function $f_{1,J}(z)$ is defined by the Stieltjes measure $\gamma_{1,J}(u)$ containing a point mass (i.e. $\gamma_{1,J}(0_+) - \gamma_{1,J}(0_-) > 0$) at the origin

$$f_{1,J}(z) = \int_0^{\infty} \frac{d\gamma_{1,J}(u)}{1 + zu}, \quad \gamma_{1,J}(u) = \sum_{n=0}^J C_{n,J}^{(1)} H(u - U_{n,J}^{(1)}), \quad U_{0,J}^{(1)} = 0, \quad (1.99)$$

$$0 < C_{0,J}^{(1)}, \quad 0 < C_{n-1,J}^{(1)}, \quad 0 < C_{n,J}^{(1)}; \quad 0 < U_{n-1,J}^{(1)} < U_{n,J}^{(1)} \leq \infty, \quad n = 2, 3, \dots, J$$

then $f_{2,J}(z)$ satisfying

$$f_{1,J}(z) = \frac{f_{1,J}(a)}{1 + (z - a)f_{2,J}(z)}, \quad a \in \left(-\frac{1}{U_{J,J}^{(1)}}, \infty \right) \quad (1.100)$$

is determined by $\gamma_{2,J}(u)$ containing no point mass (i.e. $\gamma_{2,J}(0_+) - \gamma_{2,J}(0_-) = 0$) at the origin

$$f_{2,J}(z) = \int_0^\infty \frac{d\gamma_{2,J}(u)}{1 + zu}, \quad \gamma_{2,J}(u) = \sum_{n=1}^J C_{n,J}^{(2)} H(u - U_{n,J}^{(2)}), \quad U_{0,J}^{(2)} > 0, \quad (1.101)$$

$$0 < C_{n-1,J}^{(2)}, \quad 0 < C_{n,J}^{(2)}, \quad 0 < U_{n-1,J}^{(2)} < U_{n-1,J}^{(1)} < U_{n,J}^{(2)} < U_{n,J}^{(1)}, \quad n = 2, \dots, J.$$

Proof. The relations (1.99) coincide with (1.84), while (1.101) with (1.85). ■

For the case $J \rightarrow \infty$ Lemmas 1.2, 1.3 and Theorem 1.6 yield immediately:

Theorem 1.7 Let $\Delta\gamma_j(0) = \gamma_j(0_+) - \gamma_j(0_-)$, $j = 1, 2$ denotes the jumps of $\gamma_j(u)$ at $u = 0$. If $f_1(z)$ is a Stieltjes function

$$f_1(z) = \int_0^\infty \frac{d\gamma_1(u)}{1 + zu}, \quad d\gamma_1(u) \geq 0, \quad (\text{resp. } \Delta\gamma_1(0) > 0), \quad (\text{resp. } \Delta\gamma_1(0) = 0) \quad (1.102)$$

then $f_2(z)$ satisfying

$$f_1(z) = \frac{f_1(a)}{1 + (z - a)f_2(z)}, \quad a \in \left(-\frac{1}{U_{J,J}^{(1)}}, \infty \right) \quad (1.103)$$

is a Stieltjes function as well

$$f_2(z) = \int_0^\infty \frac{d\gamma_2(u)}{1 + zu}, \quad d\gamma_2(u) \geq 0, \quad (\text{resp. } \Delta\gamma_2(0) = 0), \quad (\text{resp. } \Delta\gamma_2(0) > 0). \quad (1.104)$$

Proof. For $J \rightarrow \infty$ the relations (1.99) converge to (1.102), while (1.101) to (1.104). ■

Conclusion 1.8 From (1.102_{2,3}) and (1.104_{2,3}), it follows:

$$\text{If } \Delta\gamma_1(0) > 0 \text{ then } f_1(\infty) > 0 \text{ and } \Delta\gamma_2(0) = 0 \text{ and } f_2(\infty) = 0, \quad (1.105)$$

$$\text{If } \Delta\gamma_1(0) = 0 \text{ then } f_1(\infty) = 0 \text{ and } \Delta\gamma_2(0) > 0 \text{ and } f_2(\infty) > 0.$$

The relations (1.105) obtained in [54] and rigorously proved in [27] justify the existence of S -continued fraction expansions of Stieltjes functions. Now we can state the following:

Theorem 1.9 Let $\Delta\gamma_j(0) = \gamma_j(0_+) - \gamma_j(0_-)$, $j = 1, 2$ denotes the jumps of $\gamma_j(u)$ at $u = 0$. If $f_1(z)$ is a Stieltjes function

$$f_1(z) = \int_0^\infty \frac{d\gamma_1(u)}{1 + zu}, \quad d\gamma_1(u) \geq 0, \quad \Delta\gamma_1(0) = 0 \quad (1.106)$$

then $f_2(z)$ satisfying

$$f_1(z) = \frac{f_1(a)}{1 + (z-a)\frac{f_1(a)}{\varphi_1(\infty)} + (z-a)f_2(z)}, \quad a \in (0, \infty) \quad (1.107)$$

is a Stieltjes function as well

$$f_2(z) = \int_0^{\infty} \frac{d\gamma_2(u)}{1+zu}, \quad d\gamma_2(u) \geq 0, \quad \Delta\gamma_2(0) = 0, \quad (1.108)$$

where

$$\varphi_1(\infty) = \lim_{z \rightarrow \infty} z f_1(z). \quad (1.109)$$

Proof. The proof of Theorem 1.9 can be proceeded analogously to the proof of Theorem 1.7. ■

Conclusion 1.10 From (1.106_{2,3}) and (1.108_{2,3}), it follows:

$$\text{If } \Delta\gamma_1(0) = 0 \text{ then } f_1(\infty) = 0 \text{ and } \Delta\gamma_2(0) = 0 \text{ and } f_2(\infty) = 0. \quad (1.110)$$

The results (1.110) justify the existence of the so called T -expansions of Stieltjes functions investigated in Chapter 3. The case $a = 0$ has been investigated earlier by Tokarzewski [54, 55] and Gilewicz *et al.* [27, 28]. It is worth noting that for $\varphi_1(\infty) = \infty$ Theorem 1.9 reduces to Theorem (1.7).

1.5.2 Linear fractional transformation of $f_2(z)$ to $f_1(z)$

Now we assume that the Stieltjes function $f_{2,J}(z)$ and the value $f_{1,J}(a) \in (0, \infty)$ are known.

Lemma 1.11 If the functions (1.84) and (1.85) are interrelated by S -linear fractional transformation

$$f_{1,J}(z) = \frac{f_{1,J}(a)}{1 + (z-a)f_{2,J}(z)}, \quad f_{1,J}(a) > 0, \quad a \in \left(-\frac{1}{U_{J,J}^{(2)}}, \infty\right) \quad (1.111)$$

then $U_{n,J}^{(1)}, C_{n,J}^{(1)}$ depend on $U_{n,J}^{(2)}, C_{n,J}^{(2)}$ as follows

$$U_{n,J}^{(1)} = -\frac{1}{Z_{n,J}^{(2)}}, \quad n = 0, 1, \dots, J, \quad (1.112)$$

$$C_{0,J}^{(1)} = \begin{cases} -\frac{f_{1,J}(a)}{Z_{0,J}^{(2)}\beta_2'(Z_{0,J}^{(2)})} & \text{if } U_{0,J}^{(2)} = 0, \\ \frac{f_1(a)}{1 + \sum_{n=0}^J \frac{C_{n,J}^{(2)}}{U_{n,J}^{(2)}}} & \text{if } U_{0,J}^{(2)} = \infty \end{cases}, \quad C_{n,J}^{(1)} = -\frac{f_{1,J}(a)}{Z_{n,J}^{(2)}\beta_2'(Z_{n,J}^{(2)})}, \quad n = 1, 2, \dots, J. \quad (1.113)$$

The inequalities (1.84_{2,3}) are immediate consequence of the relations (1.113) and (1.85_{2,3}). Here $\beta_2'(z)$ is determined by

$$\beta_2'(z) = \sum_{n=0}^J \frac{C_{n,J}^{(2)}}{1 + U_n^{(2)}z} - (z-a) \sum_{n=0}^J \frac{C_{n,J}^{(2)}U_{n,J}^{(2)}}{(1 + U_{n,J}^{(2)}z)^2}, \quad (1.114)$$

while $Z_{n,J}^{(2)}$ satisfies: if $U_{0,J}^{(2)} = 0$ then

$$1 + (Z_{k,J}^{(2)} - a) \sum_{n=0}^J \frac{C_{n,J}^{(2)}}{1 + U_{n,J}^{(2)} Z_{k,J}^{(2)}} = 0, \quad -\infty < Z_{0,J} < Z_{1,J} < \dots < Z_{J,J} < 0 \quad (1.115)$$

and if $U_{0,J}^{(2)} = \infty$ then

$$Z_{0,J}^{(2)} = -\infty, \quad 1 + (Z_{k,J}^{(2)} - a) \sum_{n=1}^J \frac{C_{n,J}^{(2)}}{1 + U_{n,J}^{(2)} Z_{k,J}^{(2)}} = 0, \quad -\infty < Z_{1,J} < \dots < Z_{J,J} < 0. \quad (1.116)$$

Proof. With the help of (1.84)-(1.85) let us rewrite (1.111) as follows

$$\beta_{2,J}(z) = 1 + (z - a) \sum_{n=0}^J \frac{C_{n,J}^{(2)}}{1 + U_{n,J}^{(2)} z} = f_{1,J}(a) \left(\sum_{n=0}^N \frac{C_{n,J}^{(1)}}{1 + U_{n,J}^{(1)} z} \right)^{-1}. \quad (1.117)$$

By differentiating both sides of (1.117) one obtains

$$\begin{aligned} \beta'_{2,J}(z) &= \sum_{n=0}^J \frac{C_{n,J}^{(2)}}{1 + U_{n,J}^{(2)} z} - (z - a) \sum_{n=0}^J \frac{C_{n,J}^{(2)} U_{n,J}^{(2)}}{(1 + U_{n,J}^{(2)} z)^2} \\ &= f_1(a) \sum_{n=0}^N \frac{C_{n,J}^{(1)} U_{n,J}^{(1)}}{(1 + U_{n,J}^{(1)} z)^2} \left(\sum_{n=0}^N \frac{C_{n,J}^{(1)}}{1 + U_{n,J}^{(1)} z} \right)^{-2} > 0. \end{aligned} \quad (1.118)$$

The analytical function $\beta_{2,J}(z) = 1 + (z - a)f_{2,J}(z)$ includes the Stieltjes one $f_{2,J}(z)$, cf. (1.117) and (1.85). On account of that the roots $Z_{k,J}^{(2)}$ of the equations (1.115)-(1.116) are negative. Moreover, from the same reason $\beta'_{2,J}(Z_{k,J}^{(2)})$ take positive values (cf. (1.85) and (1.117)). Hence the relations (1.112) follow from (1.115), (1.116) and (1.117), while (1.113) is a consequence of (1.117) and (1.118). The proof is complete. ■

Example 1.12 Consider the rational function

$$f_{2,3}(z) = \frac{0.3765}{1} + \frac{0.0134}{1 + 0.3778z} + \frac{0.0161}{1 + 0.5925z} + \frac{0.0082}{1 + 0.8685z}, \quad (1.119)$$

$$a = 1, \quad U_{0,3}^{(2)} = 0, \quad f_{1,3}(1) = 0.7321.$$

From (1.95)-(1.115), it follows

$$Z_{0,3}^{(2)} = -3.0000, \quad Z_{1,3}^{(2)} = -2.0000, \quad Z_{2,3}^{(2)} = -1.3333, \quad Z_{3,3}^{(2)} = -1.0000, \quad (1.120)$$

$$U_{0,3}^{(1)} = 0.3330, \quad U_{1,3}^{(1)} = 0.5000, \quad U_{2,3}^{(1)} = 0.7500, \quad U_{3,3}^{(1)} = 1.0000, \quad (1.121)$$

$$C_{0,3}^{(1)} = 0.1667, \quad C_{1,3}^{(1)} = 0.2500, \quad C_{2,3}^{(1)} = 0.3334, \quad C_{3,3}^{(1)} = 0.5000. \quad (1.122)$$

By substituting (1.95)-(1.97) into (1.85) one obtains

$$f_{1,3}(z) = \frac{0.1667}{1 + 0.3334z} + \frac{0.25}{1 + 0.5z} + \frac{0.3334}{1 + 0.75z} + \frac{0.5}{1 + z}. \quad (1.123)$$

The inequalities (1.84_{2,3}) and (1.85_{2,3}) are satisfied.

Now on account of Lemma (1.11) we can state (cf. Theorem 1.7):

Theorem 1.13 *Let $\Delta\gamma_j(0) = \gamma_j(0_+) - \gamma_j(0)$, $j = 1, 2$ denotes the jumps of $\gamma_j(u)$ at $u = 0$. If $f_2(z)$ is a Stieltjes function*

$$f_2(z) = \int_0^{\infty} \frac{d\gamma_2(u)}{1+zu}, \quad d\gamma_2(u) \geq 0, \quad (\text{resp. } \Delta\gamma_2(0) > 0), \quad (\text{resp. } \Delta\gamma_2(0) = 0) \quad (1.124)$$

then $f_1(z)$ satisfying

$$f_1(z) = \frac{f_1(a)}{1+(z-a)f_2(z)}, \quad f_1(a) \in (0, \infty), \quad a \in \mathbb{R} \quad (1.125)$$

is a Stieltjes function as well

$$f_1(z) = \int_0^{\infty} \frac{d\gamma_1(u)}{1+zu}, \quad d\gamma_1(u) \geq 0, \quad (\text{resp. } \Delta\gamma_1(0) = 0), \quad (\text{resp. } \Delta\gamma_1(0) > 0). \quad (1.126)$$

Proof. To prove Theorem (1.13) it suffices to represent $f_2(z)$ and $f_1(z)$ appearing in (1.124)-(1.126) by means of sums of simple fractions (1.72) and uses Lemma 1.3 to justify the relations (1.126). ■

Conclusion 1.14 *From (1.10_{2,3}) and (1.10_{4,3}), it follows:*

$$\text{If } \Delta\gamma_2(0) = 0 \text{ and } f_2(\infty) = 0 \text{ and } \Delta\gamma_1(0) > 0 \text{ then } f_1(\infty) > 0, \quad (1.127)$$

$$\text{If } \Delta\gamma_2(0) > 0 \text{ and } f_2(\infty) > 0 \text{ and } \Delta\gamma_1(0) = 0 \text{ then } f_1(\infty) = 0.$$

Now we can state the following:

Theorem 1.15 *Let $\Delta\gamma_j(0) = \gamma_j(0_+) - \gamma_j(0_-)$, $j = 1, 2$ denotes the jumps of $\gamma_j(u)$ at $u = 0$. If $f_2(z)$ is a Stieltjes function*

$$f_2(z) = \int_0^{\infty} \frac{d\gamma_2(u)}{1+zu}, \quad d\gamma_2(u) \geq 0, \quad \Delta\gamma_2(0) = 0 \quad (1.128)$$

then $f_1(z)$ satisfying

$$f_1(z) = \frac{f_1(a)}{1+(z-a)\frac{f_1(a)}{\varphi_1(\infty)} + (z-a)f_2(z)}, \quad f_1(a) \in (0, \infty), \quad a \in \mathbb{R} \quad (1.129)$$

is a Stieltjes function as well

$$f_1(z) = \int_0^{\infty} \frac{d\gamma_1(u)}{1+zu}, \quad d\gamma_1(u) \geq 0, \quad \Delta\gamma_1(0) = 0, \quad (1.130)$$

where

$$\varphi_1(\infty) = \lim_{z \rightarrow \infty} z f_1(z) < \infty. \quad (1.131)$$

Proof. The proof of Theorem 1.15 is analogous to the proof of Theorem 1.9. ■

1.5.3 Properties of Stieltjes functions undergoing S - and T - linear fractional transformations

Let us introduce the sets of Stieltjes functions f containing:

Γ – all Stieltjes functions (cf. Definition 1.1))

$$\Gamma = \left\{ f ; f(z) = \int_0^{\infty} \frac{d\gamma(u)}{1+zu}, d\gamma(u) \geq 0 \right\}; \quad (1.132)$$

Γ_a^1 –the Stieltjes functions satisfying $f(a) = g \in \mathbb{R}$

$$\Gamma_a^1 = \left\{ f ; f(z) = \int_0^{\infty} \frac{d\gamma(u)}{1+zu}, f(a) = g, d\gamma(u) \geq 0 \right\}; \quad (1.133)$$

$\Gamma_{a,\infty}^{1,1}$ –the Stieltjes functions taking values $f(a) = g \in \mathbb{R}$ and $f(\infty) = d < g$

$$\Gamma_{a,\infty}^{1,1} = \left\{ f ; f(z) = \int_0^{\infty} \frac{d\gamma_1(u)}{1+zu}, f_1(a) = g, f_1(\infty) = d, d\gamma_1(u) \geq 0 \right\}. \quad (1.134)$$

Now we state the most important property of the two Stieltjes functions f_1 and f_2 inter-relating by S - or T -fractional transformations, cf. (1.75) and (1.76).

Theorem 1.16 *There is one to one correspondence between Stieltjes functions*

$$f_1 \in \Gamma_a^1 \text{ and } f_2 \in \Gamma \quad (f_1 \in \Gamma_{a,\infty}^{1,1} \text{ and } f_2 \in \Gamma) \quad (1.135)$$

satisfying the S -fractional transformation (1.75) (T - fractional transformation (1.76)).

Proof. It suffices to proceed the proof for S -fractional transformation only, cf. (1.75). For T -transformation (1.76) the proof is analogous. Let introduce the sets of rational Stieltjes functions $\overset{J}{\Gamma}$ and $\overset{J}{\Gamma}_a^1$, $J = 0, 1, 2, \dots$

$$\overset{J}{\Gamma} = \{f_{2,J} ; f_{2,J}(z) \text{ defined by (1.85)}\}, \overset{J}{\Gamma}_a^1 = \{f_{1,J} ; f_{1,J}(z) \text{ defined by (1.84)}\}. \quad (1.136)$$

On account of Lemma 1.2 the sets Γ (1.132) and Γ_a^1 (1.133) include the sets $\overset{J}{\Gamma}$ (1.136₁) and $\overset{J}{\Gamma}_a^1$ (1.136₂), i.e.

$$\Gamma = \overset{0}{\Gamma} \cup \overset{1}{\Gamma} \cup \dots \cup \overset{J}{\Gamma} \quad \text{and} \quad \Gamma_a^1 = \overset{0}{\Gamma}_a^1 \cup \overset{1}{\Gamma}_a^1 \cup \dots \cup \overset{J}{\Gamma}_a^1, J \rightarrow \infty. \quad (1.137)$$

Theorem 1.16 is valid for any fixed J (cf. Lemmas 1.4 and 1.11)

$$f_1 \in \overset{J}{\Gamma}_a^1 \text{ and } f_2 \in \overset{J}{\Gamma}, J = 0, 1, 2, 3, \dots \quad (1.138)$$

Thus it is valid for $f_2 \in \Gamma$ and $f_1 \in \Gamma_a^1$ as well, cf. (1.137). The proof is complete. ■

Theorem 1.16 is new. It will be used to prove that the rational estimations of a Stieltjes function obtained in the present work are the best.

1.6 Elementary estimates of a Stieltjes function

At first we prove the following lemma useful for estimating of Stieltjes functions from the incomplete power series.

Lemma 1.17 *A Stieltjes function $f(z)$ defined by*

$$f(z) = \int_0^{1/\rho} \frac{d\gamma_0(u)}{1+zu} \quad (1.139)$$

has the Stieltjes integral representation

$$f(z) = \int_0^{1/(\rho+w)} \frac{d\gamma_w(u)}{1+(z-w)u}, \quad w > -\rho, \quad (1.140)$$

where

$$d\gamma_w(u) = (1-uw)d\gamma_0[u/(1-uw)]. \quad (1.141)$$

Proof. By making in (1.139) the change of variables

$$v = \frac{u}{1+wu} \quad (1.142)$$

we obtain (cf. [6, Lemma 17.1])

$$f(z+w) = \int_0^{1/\rho} \frac{d\gamma_0(u)}{1+(z+w)u} = \int_0^{1/(\rho+w)} \frac{(1-vw)d\gamma_0(v/(1-vw))}{1+zv}. \quad (1.143)$$

From (1.143) the Stieltjes integral representation (1.140)-(1.141) follows at once. ■

Definition 1.18 *The Stieltjes function $\bar{f}(z)$*

$$\bar{f}(z) = \int_0^{\infty} \frac{d\bar{\alpha}(u)}{1+zu}, \quad d\bar{\alpha}(u) > 0, \quad z \in \mathbb{C} \setminus [-\infty, 0] \quad (1.144)$$

we call the normalized one if

$$\bar{f}(0) = 1. \quad (1.145)$$

Note that the Stieltjes integral (1.144) is a particular case of (1.140, $w = 0$ and $\rho = 0$). According to Definition (1.18) the ratio $f(z+x)/f(x)$ is the normalized Stieltjes function $\bar{f}(z)$ (see Fig. 1.4)

$$\bar{f}(z) = \frac{f(z+x)}{f(x)}, \quad z \in \mathbb{C} \setminus [-\infty, 0], \quad -\rho < x. \quad (1.146)$$

We now turn our attention to the problem of computing the range of possible complex values of $f(z)$ subject to (1.145). By using (1.140) we can rewrite (1.144) as the following equality

$$\bar{f}(z) = \int_0^1 \frac{d\bar{\gamma}(u)}{1+(z-1)u}, \quad d\bar{\gamma}(u) = (1-u)d\bar{\alpha}[u/(1-u)], \quad 0 \leq z \leq \infty, \quad (1.147)$$

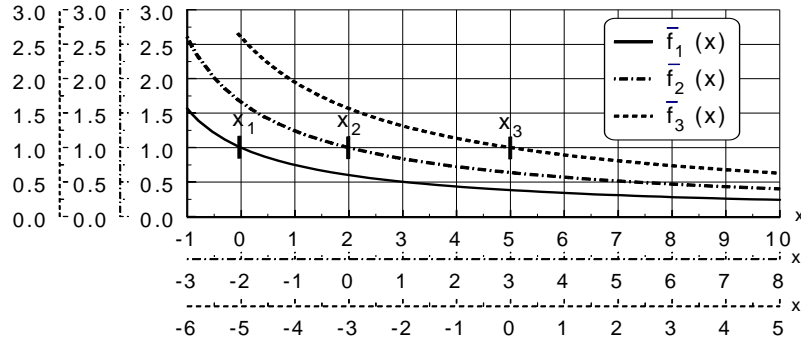


Fig. 1.4 The normalized Stieltjes functions $\bar{f}_j(x) = (f(x + x_j)/f(x_j)), j = 1, 2, 3$, where $f(x) = (1 + 2.5(\ln((1 + 0.1x)/(1 + 0.5x)))/x)/x$.

where for $z = 0$ we have

$$\bar{f}(0) = \int_0^1 \frac{d\bar{\gamma}(u)}{1-u} = 1. \tag{1.148}$$

By the equation (1.148)

$$d\bar{\omega}(u) = \frac{d\bar{\gamma}(u)}{1-u} \tag{1.149}$$

is also an allowable measure in a Stieltjes integral with the constraint

$$\int_0^1 d\bar{\omega}(u) = 1. \tag{1.150}$$

Thus for a fixed z we can write

$$\bar{f}(z, \bar{\omega}(u)) = \int_0^1 \frac{(1-u)}{1+(z-1)u} d\bar{\omega}(u), \tag{1.151}$$

where $d\bar{\omega}$ is an arbitrary, nonnegative-definite, normalized measure. From (1.151), it follows at once, that if H_1 and H_2 are the possible values of $\bar{f}(z, \bar{\omega}(u))$, then $\alpha H_1 + (1 - \alpha)H_2, 0 \leq \alpha \leq 1$ are too. On account of that if $\bar{\omega}_1$ and $\bar{\omega}_2$ are allowed measures in (1.151), then so, too, is $\alpha\bar{\omega}_1 + (1 - \alpha)\bar{\omega}_2$. Consequently, the range of $\bar{f}(z)$ is a convex region bounded by the curve consisting of the arc of the circle

$$\left\{ w \in \mathbb{C} : w = \frac{1-u}{1+(z-1)u}, 0 \leq u \leq 1 \right\} \tag{1.152}$$

and of the segment lying on the real axis

$$\{x \in \mathbb{R} : x = 1 + u, -1 \leq u \leq 0\}. \tag{1.153}$$

Lines (1.152) and (1.153) are drawn in Fig. 1.5. The ends of the arc (1.152) and of the segment (1.153) are denoted by AB , respectively.

Definition 1.19 For a fixed $z \in \mathbb{C} \setminus [-\infty, 0]$ we call in turn: 1)

$$F_1(z, u) = \begin{cases} 1 + u & \text{if } -1 \leq u \leq 0, \\ \frac{1-u}{1+(z-1)u} & \text{if } 0 \leq u \leq 1, \end{cases} \tag{1.154}$$

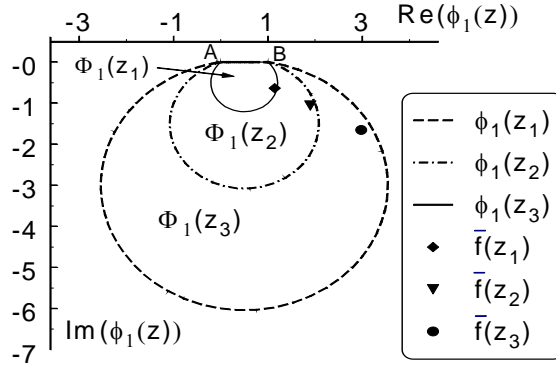


Fig. 1.5 The elementary boundaries $\phi_1(z_j)$, the elementary inclusion regions $\Phi_1(z_j)$, the values of the normalized Stieltjes functions $\bar{f}(z_j) = \frac{f(z_j+x_j)}{f(x_j)}$, $j = 1, 2, 3$; $f(z) = \frac{1}{z} \left(1 + \frac{2.5}{z} \ln \frac{1+0.1z}{1+0.5z}\right)$, $x_1 = 0$, $x_2 = 2$, $x_3 = 5$, $z_1 = -1 + i$, $z_2 = -3 + i$, $z_3 = -6 + i$.

the elementary bounding function; 2)

$$\Phi_1(z) = \{w \in \mathbb{C} : w = vF_1(z, u); \quad -1 \leq u \leq 1, \quad 0 \leq v \leq 1\}, \quad (1.155)$$

the elementary inclusion region; 3)

$$\phi_1(z) = \{w \in \mathbb{C} : w = F_1(z, u); \quad -1 \leq u \leq 1\}, \quad (1.156)$$

the elementary complex boundary; 4)

$$\bar{f}(z) = \frac{f(z+x)}{f(x)} \in \Phi_1(z), \quad x \in (-\varrho, \infty), \quad (1.157)$$

the elementary inclusion relation.

Corollary 1.20 *The elementary estimations of $\bar{f}(z)$ given by (1.154), (1.155) and (1.156) are the best.*

Proof. The bounding function $F_1(z, u)$ (1.154) consists of the parametric Stieltjes functions

$$F_1(z, u) = \begin{cases} 1 + u = \int_0^{\infty} \frac{(1+u) dH(\tau)}{1+z\tau}, & -1 \leq u \leq 0, \\ \frac{1-u}{1+(z-1)u} = \int_0^{\infty} \frac{dH(\tau - \frac{u}{1-u})}{1+z\tau}, & 0 \leq u \leq 1. \end{cases} \quad (1.158)$$

Since expression (1.158) defines via (1.156) the complex boundary $\phi_1(z)$ then the S -estimations (1.158), (1.154)-(1.156) evaluated from the input data $\bar{f}(0) = 1$ are the best. ■

By way of illustration of the Definition 1.19 the elementary inclusion regions $\Phi_1(z_j)$, the complex boundaries $\phi_1(z_j)$ and the values of $\bar{f}(z_j) = f(z_j+x_j)/f(x_j)$, $j = 1, 2, 3$ are evaluated and depicted in Fig. 1.5.

1.7 First order estimates of a Stieltjes function

By starting from the inclusion relation given by (1.157) we arrive first at

$$\frac{f_1(z)}{f_1(x)} \in \Phi_1(z - x) \tag{1.159}$$

and next at

$$f_1(z) \in f_1(x)\Phi_1(z - x) = \{w \in \mathbb{C} : w = Zf_1(x); Z \in \Phi_1(z - x)\}. \tag{1.160}$$

Now we introduce the definitions of $F_{1,1}(z, u)$, $\Phi_{1,1}(z)$ and $\phi_{1,1}(z)$ estimating $f_1(z)$ from the given values $f_1(x)$, cf. (1.154)-(1.157) and (1.159)-(1.160).

Definition 1.21 For a fixed $z \in \mathbb{C} \setminus [-\infty, -\varrho]$ we call in turn: 1)

$$F_{1,1}(z, u) = f_1(x)F_1(z - x, u), \quad x \in \mathbb{R}, \tag{1.161}$$

the first order bounding function; 2)

$$\Phi_{1,1}(z) = \{w \in \mathbb{C} : w = vF_{1,1}(z, u); -1 \leq u \leq 1, 0 \leq v \leq 1\}, \tag{1.162}$$

the first order inclusion region; 3)

$$\phi_{1,1}(z) = \{w \in \mathbb{C} : w = F_{1,1}(z, u); -1 \leq u \leq 1\}, \tag{1.163}$$

the first order boundary; 4)

$$f_1(z) \in \Phi_{1,1}(z), \quad z \in \mathbb{C} \setminus [-\infty, x], \tag{1.164}$$

the first order inclusion relation.

Corollary 1.22 The first order estimations of $\bar{f}(z)$ given by (1.154), (1.155) and (1.156) are the best.

Proof. Let us substitute in (1.161)-(1.163) new variable $z = y + x$. We obtain

$$F_{1,1}(y, u) = \varphi_1(0)F_1(y, u). \tag{1.165}$$

From Corollary 1.20 and the relations (1.161)-(1.163), it follows Corollary 1.22 at once ■

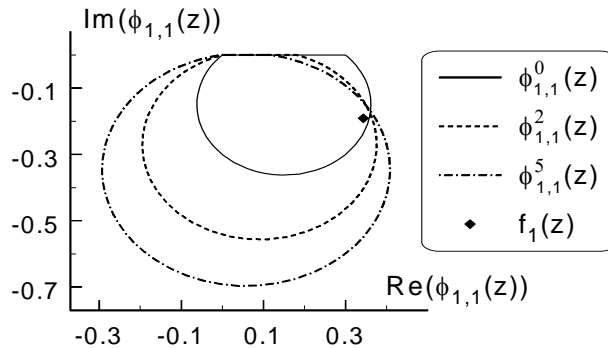


Fig. 1.6 The first order complex boundaries $\phi_{1,1}^0(z)$, $\phi_{1,1}^2(z)$ and $\phi_{1,1}^5(z)$ for the Stieltjes function $f_1(z) = \frac{1}{z} \left(1 + \frac{1}{z} 2.5 \ln \frac{1+0.1z}{1+0.5z} \right)$, where $z = -1 + i$.

As an illustrative examples of (1.161)-(1.163) let us consider the input data

$$\begin{aligned} z &= -1 + i; \quad x_1 = 0, \quad f_1(0) = 0.30; \\ x_2 &= 2, \quad f_1(2) = 0.18; \quad x_3 = 5, \quad f_1(5) = 0.12 \end{aligned} \quad (1.166)$$

computed from the Stieltjes function $f_1(z)$

$$f_1(z) = \frac{1}{z} \left(1 + \frac{1}{z} 2.5 \ln \frac{1 + 0.1z}{1 + 0.5z} \right). \quad (1.167)$$

For $f_1(z)$ (1.167), due to (1.163) and (1.161) the first order boundaries $\phi_{1,1}^{x_j}(z)$, $j = 1, 2, 3$ are equal to

$$\phi_{1,1}^0(z) = \{w = 0.30(1+u); -1 \leq u \leq 0\} \cup \left\{ w = \frac{0.30(1-u)}{1+(z-1)u}; 0 \leq u \leq 1 \right\}, \quad (1.168)$$

$$\phi_{1,1}^2(z) = \{w = 0.18(1+u); -1 \leq u \leq 0\} \cup \left\{ w = \frac{0.18(1-u)}{1+(z-3)u}; 0 \leq u \leq 1 \right\}, \quad (1.169)$$

$$\phi_{1,1}^5(z) = \{w = 0.12(1+u); -1 \leq u \leq 0\} \cup \left\{ w = \frac{0.12(1-u)}{1+(z-6)u}; 0 \leq u \leq 1 \right\}. \quad (1.170)$$

For $z = -1 + i$ the bounds $\phi_{1,1}^0(z)$, $\phi_{1,1}^2(z)$, $\phi_{1,1}^5(z)$ and $f_1(z)$ (1.167) are evaluated and depicted in Fig. 1.6. Note that the following inclusion relations

$$f_1(-1+i) \in \Phi_{1,1}^0(-1+i), \quad f_1(-1+i) \in \Phi_{1,1}^2(-1+i), \quad f_1(-1+i) \in \Phi_{1,1}^5(-1+i) \quad (1.171)$$

are satisfied.

1.8 Low order estimates of a Stieltjes function

Let us denote the given values of $f_1(z)$ as follows

$$f_1(\xi) = \eta, \quad f_1(x) = g_1, \quad \xi, \eta, x, g_1 \in \mathbb{R}, \quad \xi < x, \quad g_1 < \eta. \quad (1.172)$$

The first order bounding functions $F_{1,1}(z, u)$ computed from (1.172) take the form (see (1.161) and (1.172))

$$F_{1,1}(z, u) = f_1(\xi)F_1(z - \xi, u) = \eta F_1(z - \xi, u). \quad (1.173)$$

Consider a linear fractional transformation of $f_1(z)$ to $f_2(z)$

$$f_1(z) = \frac{f_1(x)}{1+(z-x)f_2(z)} = \frac{f_1(x)}{1+(z-x)f_2(\xi)\bar{f}_2(z)} = \frac{f_1(x)}{1+(z-x)w_2\bar{f}_2(z)}, \quad (1.174)$$

where $\bar{f}_2(z)$ is a normalized Stieltjes function, cf. Definition 1.18 and Theorem (1.7). Hence on account Definition (1.21) the first order bounding function $F_{1,2}(z, u)$ estimating $f_2(z)$ is equal to (cf.(1.174))

$$F_{1,2}(z, u) = F_1(z - \xi, u)f_2(\xi) = F_1(z - \xi, u)w_2, \quad (1.175)$$

where we introduced

$$w_2 = f_2(\xi). \quad (1.176)$$

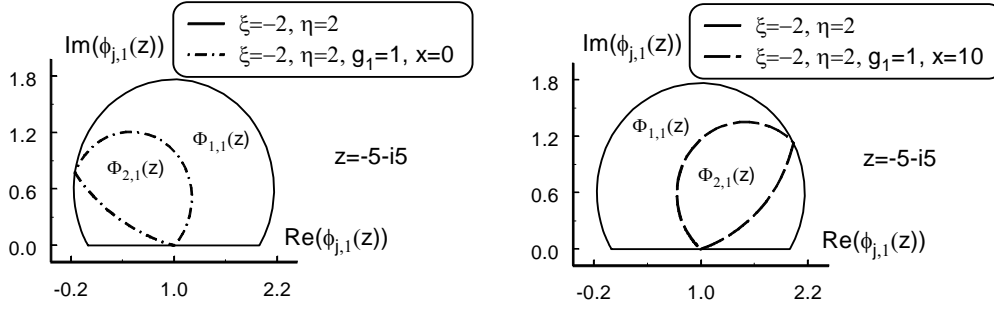


Fig. 1.7 The inclusion regions $\Phi_{j,1}(z)$ and the complex boundaries $\phi_{j,1}(z)$, $j = 1, 2$ for the Stieltjes function $f_1(z)$ evaluated from the values $f_1(\xi) = \eta$ and $f_1(x) = g_1$, $\xi < x$. Note that the inclusion relation $\Phi_{2,1}(z) \subset \Phi_{1,1}(z)$ predicted by (1.185) is satisfied.

1.8.1 Inclusion regions depending on P .

By replacing in (1.174) $f_2(z)$ by its estimation $F_{1,2}(z, u)$ one obtains the bounding function of the second order $F_{2,1}(z, u)$

$$F_{2,1}(z, u) = \frac{g_1}{1 + (z - x)F_{1,2}(z, u)}. \quad (1.177)$$

On account of (1.174) and (1.172) we have

$$F_{2,1}(\xi, 0) = \frac{g_1}{1 + (\xi - x)F_{1,2}(\xi, 0)} = \frac{g_1}{1 + (\xi - x)w_2F_1(0, 0)} = \eta. \quad (1.178)$$

Since $F_1(0, 0) = 1$ the relations (1.178) yield

$$w_2 = \frac{(\eta - g_1)}{\eta(x - \xi)}. \quad (1.179)$$

Thus the second order bounding function $F_{2,1}(z, u)$ takes the explicit form (cf. (1.177))

$$F_{2,1}(z, u) = \frac{g_1}{1 + (z - x)\frac{(\eta - g_1)}{\eta(x - \xi)}F_1(z - \xi, u)}. \quad (1.180)$$

By equating (1.173) with (1.180) one obtains the relation

$$F_{1,1}(z, u) = F_{2,1}(z, v), \quad -1 \leq u, v \leq 1 \quad (1.181)$$

determining the points lying on the curves $F_{1,1}(z, u)$ and $F_{2,1}(z, v)$ simultaneously. Let us rewrite (1.181) as follows

$$\eta F_1(z - \xi, u) = \frac{g_1}{1 + (z - x)\frac{(\eta - g_1)}{\eta(x - \xi)}F_1(z - \xi, v)}, \quad u, v \in \mathbb{R}. \quad (1.182)$$

Two solutions of (1.182) exist

$$u_1 = -\frac{\eta - g_1}{\eta}, \quad v_1 = 1 \quad \text{and} \quad u_2 = \frac{\eta - g_1}{(x - \xi)g_1 + \eta - g_1}, \quad v_2 = 0. \quad (1.183)$$

Lemma 1.23 For $z \in \mathbb{C} \setminus [-\infty, \xi]$, $x \in \mathbb{R} \setminus [-\infty, \xi]$, $\xi < x < \infty$ and $g_1 < \eta$ we have:
The second order bounding function $F_{2,1}(z, u)$ touches the first order one $F_{1,1}(z, u)$ at two points (see (1.183))

$$F_{1,1}\left(z, -\frac{\eta - g_1}{\eta}\right) = F_{2,1}(z, 1) \text{ and } F_{1,1}\left(z, \frac{\eta - g_1}{(x - \xi)g_1 + \eta - g_1}\right) = F_{2,1}(z, 0). \quad (1.184)$$

The lens-shaped inclusion regions $\Phi_{2,1}(z)$ and $\Phi_{1,1}(z)$ satisfy the relations

$$f_1(z) \in \Phi_{2,1}(z) \subset \Phi_{1,1}(z). \quad (1.185)$$

Proof. Let us consider the sets Γ_ξ^1 , Γ_x^1 and $\Gamma_{x,\xi}^{1,1}$ of Stieltjes functions f_1 defined by

$$\Gamma_\xi^1 = \left\{ f_1; f_1(z) = \int_0^\infty \frac{d\gamma_1(u)}{1 + zu}, f_1(\xi) = \eta, d\gamma_1(u) \geq 0 \right\}, \quad (1.186)$$

and

$$\Gamma_x^1 = \left\{ f_1; f_1(z) = \int_0^\infty \frac{d\gamma_1(u)}{1 + zu}, f_1(x) = g_1, d\gamma_1(u) \geq 0 \right\}, \quad (1.187)$$

and

$$\Gamma_{x,\xi}^{1,1} = \Gamma_\xi^1 \cap \Gamma_x^1. \quad (1.188)$$

The first and second order inclusion regions $\Phi_{1,1}(z)$ and $\Phi_{2,1}(z)$ are the best with respect to the given values η and g_1 . Hence on account of Definition 1.21 and due to relation (1.180) we have

$$\Phi_{1,1}^{\xi,\eta}(z) = \Gamma_\xi^1(z), \quad \Phi_{2,1}^{\xi,\eta}(z) = \Gamma_{x,\xi}^{1,1}(z). \quad (1.189)$$

From (1.189) and

$$\Gamma_{x,\xi}^{1,1} \subset \Gamma_\xi^1, \quad (1.190)$$

it follows

$$\Phi_{2,1}^{\xi,\eta}(z) \subset \Phi_{1,1}^{\xi,\eta}(z). \quad (1.191)$$

The proof is complete, cf. (1.185) and (1.191). ■

To illustrate Lemma 1.23 the numerical evaluations of $\Phi_{2,1}^{\xi,\eta}(z)$ (1.173) and $\Phi_{1,1}^{\xi,\eta}(z)$ (1.180) are carried out. The results are depicted in Fig. 1.7.

1.8.2 Inclusion regions depending on ξ

Consider now the sequences of the first $\Phi_{1,1}^{\xi_j, \eta_1}(z)$ and the second $\Phi_{2,1}^{\xi_j, \eta_1}(z)$ order inclusion regions of the Stieltjes functions $f_1^{\xi_j, \eta_1}(z)$, $j = 1, 2$, respectively, cf. (1.189). We assume that both $f_1^{\xi_1, \eta_1}(z)$ and $f_1^{\xi_2, \eta_1}(z)$ satisfy the assumptions (1.172).

Lemma 1.24 For $z \in \mathbb{C} \setminus [-\infty, \xi_2]$ the inclusion relations

$$f_1^{\xi_1, \eta_1}(z) \in \Phi_{1,1}^{\xi_1, \eta_1}(z) \subset \Phi_{1,1}^{\xi_2, \eta_1}(z) \quad , \quad f_1^{\xi_1, \eta_1}(z) \in \Phi_{2,1}^{\xi_1, \eta_1}(z) \subset \Phi_{2,1}^{\xi_2, \eta_1}(z) \quad (1.192)$$

are satisfied, provided the parameters ξ_1 and ξ_2 obey the inequalities

$$\xi_1 \leq \xi_2. \quad (1.193)$$

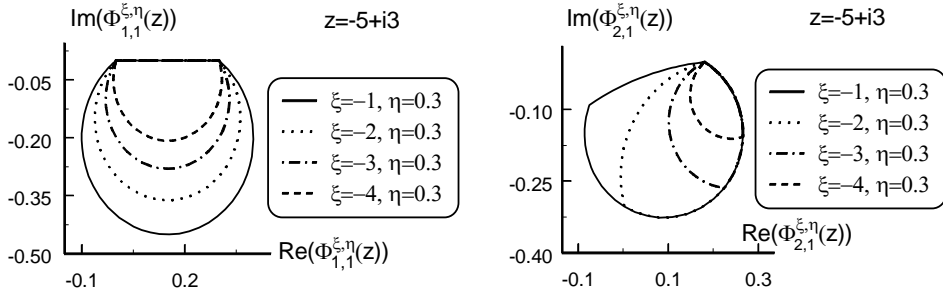


Fig. 1.8 The first $\Phi_{1,1}^{\xi,\eta}(z)$ (1.173) and the second $\Phi_{2,1}^{\xi,\eta}(z)$ (1.180) order inclusion regions constructed from the truncated power expansions $f_1(z) = \eta + O(z - \xi)$ and $f_1(z) = g_1 + O(z)$, where $g_1 = 0.1807$. Note that $\Phi_{1,1}^{\xi,\eta}(z)$ and $\Phi_{2,1}^{\xi,\eta}(z)$ satisfy the inclusion relations (1.192).

Proof. Let us rewrite the bounding function $F_{1,1}^{\xi,\eta}(x - \xi + iy, u)$ in the polar coordinates R, Θ (cf. (1.173))

$$F_{1,1}^{\xi,\eta}(x - \xi + iy, u) = \begin{cases} \eta(1 + u), & -1 < u \leq 0, \\ R \exp(i\Theta), & 0 < u \leq 1, \end{cases} \quad (1.194)$$

where

$$R = \frac{\eta(1 - u)}{(1 + ux - u\xi - u)^2 + u^2y^2}, \quad \Theta = -\arctan\left(\frac{uy}{1 + ux - u\xi - u}\right). \quad (1.195)$$

The formulae $R \exp(i\Theta(\xi)), 0 < u \leq 1$ describe the class of arcs of circles possessing common points at

$$R = 0, \Theta = 0 \text{ and } R = \eta, \Theta = 0. \quad (1.196)$$

By substituting $u = 1$ into (1.195) we obtain

$$R = 0, \Theta(\xi) = -\arctan\left(\frac{y}{x - \xi}\right). \quad (1.197)$$

From the derivative

$$\frac{\partial\Theta(\xi)}{\partial\xi} = -\frac{y}{(x - \xi)^2 + y^2}, \quad (1.198)$$

it follows the monotonicity of $\Theta(\xi)$, namely

$$\Theta(\xi) \text{ increases if } y < 0 \text{ and decreases if } y > 0. \quad (1.199)$$

Formulae (1.196) and (1.199) lead to the relation (1.192₁) at once. Similarly, on account of (1.175) one can derive the inclusion relation

$$\Phi_{1,2}^{\xi_1,\eta_1}(z) \subset \Phi_{1,2}^{\xi_2,\eta_2}(z). \quad (1.200)$$

On account of that from (1.200) and (1.180), it follows (1.192₂). ■

1.8.3 Inclusion regions depending on η

Let us explore the inclusion regions $\Phi_{1,1}^{\xi_1,\eta_j}(z)$ and $\Phi_{2,1}^{\xi_1,\eta_j}(z)$, $j = 1, 2$ estimating the Stieltjes functions $f_1^{\xi_1,\eta_1}(z)$ and $f_1^{\xi_1,\eta_2}(z)$, respectively, cf. (1.189). As in the previous subsection the functions $f_1^{\xi_1,\eta_1}(z)$ and $f_1^{\xi_1,\eta_2}(z)$ meet the requirements (1.172).

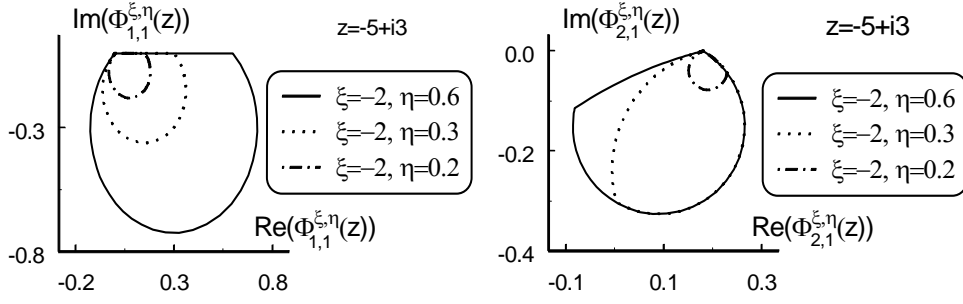


Fig. 1.9 The first $\Phi_{1,1}^{\xi,\eta}(z)$ and second $\Phi_{2,1}^{\xi,\eta}(z)$ order inclusion regions for $\xi = -2$, $\eta = 0.2, 0.3, 0.6$. Note that $\Phi_{1,1}^{\xi,\eta}(z)$ and $\Phi_{2,1}^{\xi,\eta}(z)$ confirm the inclusion relations (1.192).

Lemma 1.25 *If the parameters η_1 and η_2 satisfy the inequality*

$$\eta_1 \leq \eta_2, \quad (1.201)$$

then for $z \in \mathbb{C} \setminus [-\infty, \xi]$ the inclusion relations are satisfied

$$f_1^{\xi_1, \eta_1}(z) \in \Phi_{1,1}^{\xi_1, \eta_1}(z) \subset \Phi_{1,1}^{\xi_1, \eta_2}(z) \text{ and } f_1^{\xi_1, \eta_1}(z) \in \Phi_{2,1}^{\xi_1, \eta_1}(z) \subset \Phi_{2,1}^{\xi_1, \eta_2}(z). \quad (1.202)$$

Proof. From (1.195), it follows that for $u = 0$ and $u = 1$ we have

$$R = 0, \quad \Theta = -\arctan\left(\frac{y}{x - \xi}\right) \text{ and } R = \eta, \quad \Theta = 0. \quad (1.203)$$

For a fixed x, y, ξ the input data (1.203) uniquely determine the arc of circle (1.194₁) and the segment (1.194₂) as a function of η . From (1.203), it follows that for any fixed values of ξ, x, y

$$R(\eta) \text{ increases if } \eta \text{ increases.} \quad (1.204)$$

The relation (1.202₁) is a simple consequence of the conclusion (1.204) and the relations (1.203). Similarly one obtains

$$\Phi_{1,2}^{\xi_1, \eta_1}(z) \subset \Phi_{1,2}^{\xi_1, \eta_2}(z). \quad (1.205)$$

Hence the relation (1.202₂) is a consequence of (1.205), cf. (1.180). ■

1.8.4 Inclusion regions depending on P, ξ, η

Now we are prepared to summarize the results obtained above stating the following lemma:

Lemma 1.26 *For fixed $z \in \mathbb{C} \setminus [-\infty, \xi_2]$ and $x_1 \in \mathbb{R}$ the inclusion regions $\Phi_{P_I,1}^{\xi_1, \eta_1}(z)$ and $\Phi_{P_{II},1}^{\xi_2, \eta_2}(z)$ computed from the truncated Stieltjes series*

$$f_1^{\xi_j, \eta_j}(z) = \eta_j + O(z - \xi_j), \quad f_1^{\xi_j, \eta_j}(z) = g_1 + O(z - x_1), \quad j = 1, 2 \quad (1.206)$$

satisfy the following relations

$$f_1^{\xi_1, \eta_1}(z) \in \Phi_{P_I,1}^{\xi_1, \eta_1}(z) \subset \Phi_{P_{II},1}^{\xi_2, \eta_2}(z), \quad (1.207)$$

provided that

$$\xi_1 \leq \xi_2, \quad \eta_1 \leq \eta_2, \quad P_{II} \leq P_I. \quad (1.208)$$

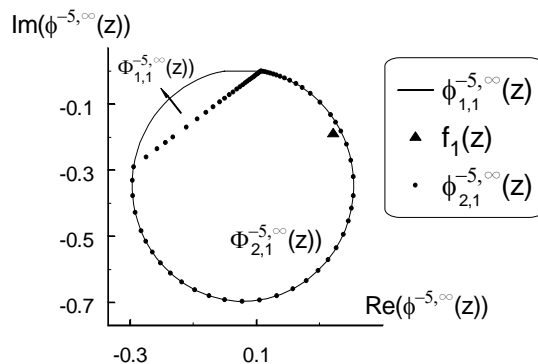


Fig. 1.10 The complex boundaries for the Stieltjes function $f_1(z) = \frac{1}{z+2}(1 + \frac{1}{z}2.5 \ln \frac{1.2+0.1z}{1.5+0.5z})$, $z = -6 + i$ evaluated from the truncated, one term series $f_1(z) = 0.11527 + O(z)$ possessing a radius of convergence $\rho \geq 5$.

Proof. From Lemmas 1.23, 1.24 and 1.25 the relations (1.207)-(1.208) follow at once. ■

As an illustration of Lemma 1.26 we consider the truncated power series $f_1(z)$ with a radius of convergence ρ not less than 5

$$f_1(z) = 0.11527 + O(z), \quad \rho \geq 5, \tag{1.209}$$

where

$$f_1(z) = \frac{1}{z+5} \left(1 + \frac{1}{z+5} 2.5 \ln \frac{1.5+0.1z}{3.5+0.5z} \right). \tag{1.210}$$

It is convenient to rewrite the input data (1.209)

$$\begin{aligned} f_1^{\xi_1, \eta_1}(z) &= g_1 + O(z), \quad f_1^{\xi_1, \eta_1}(z) = \eta_1 + O(z - \xi_1), \\ \xi_1 &= -\rho, \quad \eta_1 = \infty, \quad g_1 = 0.11527 \end{aligned} \tag{1.211}$$

and

$$\begin{aligned} f_1^{\xi_2, \eta_2}(0) &= g_1 + O(z), \quad f_1^{\xi_2, \eta_2}(z) = \eta_2 + O(z - \xi_2), \\ \xi_2 &= -5, \quad \eta_2 = \infty, \quad g_1 = 0.11527. \end{aligned} \tag{1.212}$$

The bounding functions $F_{1,1}^{-5, \infty}(z, u)$ and $F_{2,1}^{-5, \infty}(z, u)$ evaluated from (1.211) and (1.212) take the forms

$$F_{1,1}^{\xi_2, \eta_2}(z, u) = F_{1,1}^{-5, \infty}(z, u) = f_1(0)F_1(z, u), \quad F_{2,1}^{-5, \infty}(z, u) = \frac{f_1(0)}{1 + 0.2zF_1(z+5, u)}. \tag{1.213}$$

For $z = -6 + i$ the complex boundaries $\phi_{1,1}^{-5, \infty}(z)$, $\phi_{2,1}^{-5, \infty}(z)$, the inclusions regions $\Phi_{1,1}^{-5, \infty}(z)$, $\Phi_{2,1}^{-5, \infty}(z)$ and the exact value of $f_1(z)$ (1.210) are computed and depicted in Fig. 1.10.

The Theorems 1.7, 1.9 and Lemmas 1.23, 1.24, 1.25, 1.26 proved in this chapter are the starting point for developing new S - and T -Multipoint Continued Fraction Methods of an estimation of a Stieltjes function $f_1(z)$ from the power series expanded at real points (SMCFM) and in infinity (TMCFM).

Chapter 2

THE BEST ESTIMATES OF A STIELTJES FUNCTION EXPANDED AT A NUMBER OF REAL POINTS

This chapter provides a mathematical background for a S -Multipoint Continued Fraction Method (SMCFM) of an estimation of a Stieltjes function $f_1(z)$ from the truncated power series $f_1(z)$ expanded at real points x_1, x_2, \dots, x_N and ξ , where $\xi \leq \min(x_1, x_2, \dots, x_N)$ and $f_1(\xi) = \eta$.

The definitions of: S -continued fraction expansions, S -bounding functions, S -complex boundaries, S -inclusion regions and S -Padé bounds are introduced and used to developed the S -Multipoint Continued Fraction Method.

The main SMCFM tools, i.e. a recurrence S -algorithm, S -inclusion relations and S -inequalities are derived as functions of the real parameters ξ and η . For some limit values of ξ and η the S -estimates of $f_1(z)$ become the best with respect to the given input data.

The SMCFM is a first method of the theory of an approximation of Stieltjes functions that incorporates into the estimates of $f_1(z)$ the unlimited number of coefficients of the power series $f_1(z)$ expanded at several real points, cf. [6, 8, 9, 7].

In the sequel the SMCFM will be adapted for estimating of the effective transport coefficients of two-phase media.

2.1 The S -multipoint continued fraction expansions of analytical functions

Consider the truncated power expansions of an analytical function $f_1(z)$

$$\begin{aligned} f_1(z) &= f_1(z)_{x_j}^{p_j}, \quad x_j \in \mathbb{R}, \quad j = 1, 2, \dots, N; \\ f_1(z) &= f_1(z)_{\xi}^1, \quad \xi \in \mathbb{R}; \quad \xi < \min(x_j, j = 1, 2, \dots, N), \end{aligned} \quad (2.1)$$

where the abbreviations

$$f_1(z)_{x_j}^{p_j} = \sum_{i=0}^{p_j-1} c_{ij}(z-x_j)^i + O((z-x_j)^{p_j}); \quad f_1(z)_{\xi}^1 = \eta + O(z-\xi) \quad (2.2)$$

are introduced. The coefficients c_{ij} and η appearing in (2.2) are equal to

$$f_1^{(0)}(\xi) = \eta, \quad c_{ij} = c_i(x_j) = \frac{f_1^{(i)}(x_j)}{i!}, \quad f_1^{(i)}(x_j) = \left. \frac{d^i f_1(z)}{d^i(z)} \right|_{z=x_j}, \quad i = 0, 1, \dots \quad (2.3)$$

For the sake of simplicity the notations

$$f_1(z)_{\mathbf{x}}^{\mathbf{p}} = f_1(z)_{x_1, x_2, \dots, x_N, \xi}^{p_1, p_2, \dots, p_N, 1} = \{f_1(z)_{x_1}^{p_1}, f_1(z)_{x_2}^{p_2}, \dots, f_1(z)_{x_N}^{p_N}, f_1(z)_{\xi}^1\}, \quad f_1(\xi) = \eta \quad (2.4)$$

representing the relations (2.1)-(2.3) will also be used.

Remark 2.1 The components $(_{x_1, x_2, \dots, x_N, \xi}^{p_1, p_2, \dots, p_N, 1})$ of $(_{\mathbf{x}}^{\mathbf{p}})$ denote the numbers of coefficients $(p_1, p_2, \dots, p_N, 1)$ of power expansions of $f_1(z)$ available at points $(x_1, x_2, \dots, x_N, \xi)$, cf. (2.4).

Now we introduce the $L_P(x)$ -characteristic function associated with the incomplete power expansions $f_1(z)_{\mathbf{x}}^{\mathbf{p}}$.

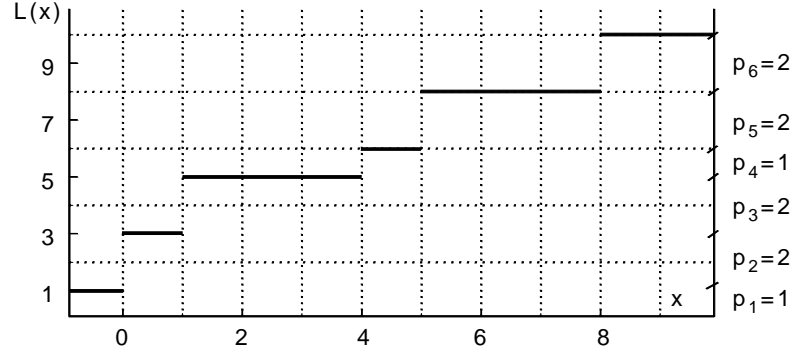


Fig. 2.1 The $L_{10}(x)$ -characteristic function generated by the truncated power expansions $f_1(z)_{\mathbf{x}}^{\mathbf{p}}$, $(\mathbf{p}) = (2, 2, 1, 2, 2, +1)$, $(\mathbf{x}) = (0, 1, 4, 5, 8, -1)$.

Definition 2.2 *The truncated power series*

$$f_1(z)_{\mathbf{x}}^{\mathbf{p}}, (\mathbf{p}) = \begin{pmatrix} p_1, p_2, \dots, p_N \\ x_1, x_2, \dots, x_N \end{pmatrix} \quad (2.5)$$

generate the non-decreasing step function $L_P(x) : \mathbb{R}^1 \rightarrow \mathbb{R}^1$

$$L_P(x) = \sum_{j=1}^N p_j H(x - x_j), P = \sum_{i=1}^N p_i, \quad (2.6)$$

called the $L_P(x)$ -characteristic function. $H(x)$ is the Heaviside step function, see (1.52).

Remark 2.3 For a fixed $s \in [1, 2, \dots, N - 1]$ and fixed $x \in [x_s, x_{s+1})$ the characteristic function $L_P(x)$ defined by the power series $f_1(z)_{\mathbf{x}}^{\mathbf{p}}$ determines the sum $p_1 + p_2 + \dots + p_s$ of the coefficients of the truncated power expansions of $f_1(z)$ at the points $x_1, x_2, \dots, x_s \leq x$, respectively.

In the sequel the non-decreasing sequences of the truncated power expansions $f_1(z)_{\mathbf{x}}^{\mathbf{p}(P)}$ will be exploited. To this end we introduce:

Definition 2.4 For fixed \mathbf{x} and $P = 1, 2, 3, \dots$ the truncated power expansions

$$f_1(z)_{\mathbf{x}}^{\mathbf{p}(P)}, (\mathbf{p}(P)) = \begin{pmatrix} p_1(P), p_2(P), \dots, p_N(P) \\ x_1, x_2, \dots, x_N \end{pmatrix}, P = \sum_{i=1}^N p_i(P) \quad (2.7)$$

we call the non-decreasing ones, if the inequalities

$$p_1(P) - p_1(P - 1) \geq 0, \dots, p_N(P) - p_N(P - k) \geq 0 \quad (2.8)$$

abbreviated by

$$\mathbf{p}(P) - \mathbf{p}(P - 1) \geq 0, P = 1, 2, 3, \dots \quad (2.9)$$

are true.

For example the sequence

$$f_1(z)_{\mathbf{x}}^{\mathbf{p}(P)}, (\mathbf{p}(2)) = \begin{pmatrix} 1, 1, 0 \\ 1, 3, -1 \end{pmatrix}, (\mathbf{p}(3)) = \begin{pmatrix} 1, 1, 1 \\ 1, 3, -1 \end{pmatrix}, (\mathbf{p}(4)) = \begin{pmatrix} 2, 1, 1 \\ 1, 3, -1 \end{pmatrix} \quad (2.10)$$

is non-decreasing, since

$$\mathbf{p}(4) - \mathbf{p}(3) = (1, 0, 0) \geq 0, \mathbf{p}(3) - \mathbf{p}(2) = (0, 0, 1) \geq 0, \quad (2.11)$$

where the notation (2.11₁) means that

$$p_1(4) - p_1(3) = 1 \geq 0, p_2(4) - p_2(3) = 0 \geq 0, p_3(4) - p_3(3) = 0 \geq 0. \quad (2.12)$$

2.1.1 Recurrence formulae for S -multipoint continued fraction expansion of a Stieltjes function

Definition 2.5 The following recurrence formula interrelating $f_1(z)$ and $f_P(z)$

$$\begin{aligned}
 f_{P_0+1}(z) &= \frac{f_{P_0+1}(x_1)}{1 + (z - x_1)f_{P_0+2}(z)}, \quad f_{P_0+2}(z) = \frac{f_{P_0+2}(x_1)}{1 + (z - x_1)f_{P_0+3}(z)}, \quad \dots, \\
 f_{P_1}(z) &= \frac{f_{P_1}(x_1)}{1 + (z - x_1)f_{P_1+1}(z)}, \quad f_{P_1+1}(z) = \frac{f_{P_1+1}(x_2)}{1 + (z - x_2)f_{P_1+2}(z)}, \\
 f_{P_1+2}(z) &= \frac{f_{P_1+2}(x_2)}{1 + (z - x_2)f_{P_1+3}(z)}, \quad \dots, \quad f_{P_2}(z) = \frac{f_{P_2}(x_2)}{1 + (z - x_2)f_{P_2+1}(z)}, \\
 &\dots\dots\dots, \\
 f_{P_{N-1}+1}(z) &= \frac{f_{P_{N-1}+1}(x_N)}{1 + (z - x_{N-1})f_{P_{N-1}+2}(z)}, \quad \dots, \quad f_{P_N}(z) = \frac{f_{P_N}(x_N)}{1 + (z - x_N)f_P(z)},
 \end{aligned}
 \tag{2.13}$$

where

$$\begin{aligned}
 f_1(z) &= f_1(z)_x^p, \quad (p) = (p_1, p_2, \dots, p_N, 1); \quad f_P(z) = f_P(z)_\xi^1 = w_P + (z - \xi), \\
 w_P &= f_P(\xi); \quad P_0 = 0, \quad P_j = \sum_{i=1}^j p_i, \quad j = 1, 2, \dots, N; \quad P = P_N + 1.
 \end{aligned}
 \tag{2.14}$$

we call the S -multipoint continued fraction expansion of $f_1(z)$ to $f_P(z)$.

In the mathematical literature the function $f_P(z)$ appearing in (2.13)-(2.14) is named the S -continued fraction tail, cf. [34, pp. 56].

Now we introduce a new notation for the S -continued fractions more convenient for estimating of the Stieltjes function $f_1(z)$ from the power expansions $f_1(z)_x^p$

$$\frac{b_1}{1 + \frac{z b_2}{1 + \frac{\dots}{1 + \frac{z b_N}{1}}}} = \bigvee_{i=1}^N \frac{b_i}{1 + z} = \frac{b_1}{1 + z} \times \frac{b_2}{1 + z} \times \dots \times \frac{b_N}{1}.
 \tag{2.15}$$

Note that the convergents of (2.15) are rational functions with the numerators, denominators of orders k , k and $k - 1, k$, respectively. By substituting in (2.13)

$$\begin{aligned}
 j = 1, \dots, P_1 : g_j &:= f_j(x_1); \quad j = P_1 + 1, \dots, P_2 : g_j := f_j(x_2); \quad \dots \\
 \dots; \quad j = P_{N-1} + 1, \dots, P_N : g_j &:= f_j(x_N); \quad w_{P_{N+1}} = w_P = f_P(\xi);
 \end{aligned}
 \tag{2.16}$$

we obtain

$$\begin{aligned}
 f_{P_0+1}(z) &= \frac{g_{P_0+1}}{1 + (z - x_2)} \times \frac{g_{P_0+2}}{1 + (z - x_2)} \times \dots \times \frac{g_{P_1}}{1 + (z - x_2)} \times \frac{f_{P_1+1}(z)}{1}, \\
 f_{P_1+1}(z) &= \frac{g_{P_1+1}}{1 + (z - x_3)} \times \frac{g_{P_1+2}}{1 + (z - x_3)} \times \dots \times \frac{g_{P_2}}{1 + (z - x_3)} \times \frac{f_{P_2+1}(z)}{1}, \\
 &\dots\dots\dots, \\
 f_{P_{N-1}+1}(z) &= \frac{g_{P_{N-1}+1}}{1 + (z - x_N)} \times \frac{g_{P_{N-1}+2}}{1 + (z - x_N)} \times \dots \times \frac{g_{P_N}}{1 + (z - x_N)} \times \frac{f_P(z)}{1}.
 \end{aligned}
 \tag{2.17}$$

On account of (2.15) the formulae (2.17) take the form

$$f_1(z) = \prod_{j=P_0+1}^{P_1} \frac{g_j}{1+(z-x_1)} \times \cdots \times \prod_{j=P_{N-1}+1}^{P_N} \frac{g_j}{1+(z-x_N)} \times \frac{f_P(z)}{1}. \quad (2.18)$$

Finally we obtain (see (2.14) and (2.16))

$$f_1(z) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1+(z-x_k)} \times \frac{f_P(z)}{1}. \quad (2.19)$$

The alternative notations for the continued fraction expansion (2.19), namely

$$\prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1+(z-x_k)} \times \frac{f_P(z)}{1} = \mathbf{S}_{P-1} f_P(z) = \prod_{k=1}^N \mathbf{S}_{P_{k-1}+1}^{P_k} f_P(z) \quad (2.20)$$

and

$$\prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1+(z-x_k)} \times \frac{f_P(z)}{1} = f_1(z, \mathbf{p}, f_P(z)), \quad (2.21)$$

$$f_1(z, \mathbf{p}, f_P(z)) = f_1\left(z, \begin{matrix} p_1, p_2, \dots, p_N, 1 \\ x_1, x_2, \dots, x_N, \xi \end{matrix}, f_P(z)\right)$$

will also be used. For an illustration of the formula (2.19) we evaluate the continued fraction expansion of $\exp(z)$ from the truncated power series

$$\exp(z)_0^1 = 1 + O(z-0), \quad \exp(z)_1^1 = 2.718 + O(z-1), \quad \exp(z)_{-1}^{+1} = 0.368 + O(z+1). \quad (2.22)$$

We obtain

$$\exp(z) = \frac{1}{1+z} \times \frac{-0.632}{1+(z-1)} \times \frac{f_3(z)}{1}, \quad f_3(z) = 0.316 + O(z+1). \quad (2.23)$$

According to (2.21), we also have

$$\exp(z) = \exp\left(z, \begin{matrix} 1, 1, +1 \\ 0, 1, -1 \end{matrix}, f_3(z)\right) = \frac{1}{1 - \frac{0.632z}{1+(z-1)f_3(z)}}. \quad (2.24)$$

2.1.2 Main properties of S -multipoint continued fraction expansions of a Stieltjes function

Now we prove a few theorems stating the most important properties of the S -multipoint continued fraction expansions of $f_1(z)$ to $f_P(z)$. We start from:

Theorem 2.6 *Let $\Delta\gamma_j(0) = \gamma_j(0_-) - \gamma_j(0_+)$ be the jumps of the Stieltjes measures $d\gamma_j(u)$, $j = 1, P$ at $u = 0$. If $f_1(z)$ is a Stieltjes function*

$$f_1(z) = \int_0^\infty \frac{d\gamma_1(u)}{1+zu}, \quad \Delta\gamma_1(0) = 0 \quad (\Delta\gamma_1(0) > 0) \quad (2.25)$$

then the tail $f_P(z)$ appearing in

$$f_1(z) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1+(z-x_k)} \times \frac{f_P(z)}{1}, \quad f_P(\xi) = w_P \quad (2.26)$$

is also a Stieltjes function

$$f_P(z) = \int_0^\infty \frac{d\gamma_P(u)}{1+zu}, \text{ where } \begin{cases} \Delta\gamma_P(0) > 0 & (\Delta\gamma_P(0) = 0) \text{ if } P \text{ is odd,} \\ \Delta\gamma_P(0) = 0 & (\Delta\gamma_P(0) > 0) \text{ if } P \text{ is even.} \end{cases} \quad (2.27)$$

Proof. By applying the linear fractional transformation (1.103) $P - 1$ times to the function $f_1(z)$ we arrive at the tail $f_P(z)$, see (2.26). The Stieltjes integral (2.27₁) and the relations (2.27₂) and (2.27₃) result directly from Theorem (1.7). ■

The next Theorem is closely connected with Theorem 2.6. It states.

Theorem 2.7 Let $\Delta\gamma_j(0) = \gamma_j(0_-) - \gamma_j(0_+)$ be the jumps of the Stieltjes measures $d\gamma_j(u)$, $j = 1, P$ at $u = 0$. If $f_P(z)$ is a Stieltjes function

$$f_P(z) = \int_0^\infty \frac{d\gamma_P(u)}{1+zu}, \quad \begin{cases} \Delta\gamma_P(0) > 0 & (\Delta\gamma_P(0) = 0) \text{ if } P \text{ is odd,} \\ \Delta\gamma_P(0) = 0 & (\Delta\gamma_P(0) > 0) \text{ if } P \text{ is even} \end{cases} \quad (2.28)$$

then $f_1(z)$ appearing in

$$f_1(z) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1+(z-x_k)} \times \frac{f_P(z)}{1}, \quad f_P(\xi) = w_P \quad (2.29)$$

is also a Stieltjes function

$$f_1(z) = \int_0^\infty \frac{d\gamma_1(u)}{1+zu}, \quad \Delta\gamma_1(0) = 0 \quad (\Delta\gamma_1(0) > 0). \quad (2.30)$$

Proof. Theorem 2.7 is a direct consequence of Theorem 1.13 ■

Theorem 2.8 Let the continued fraction expansion of a Stieltjes functions $f_1(z)$ to $f_P(z)$

$$f_1(z) = f_1\left(z, \begin{matrix} p_1, p_2, \dots, p_N, 1 \\ x_1, x_2, \dots, x_N, \xi \end{matrix}, f_P(z)\right) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1+(z-x_k)} \times \frac{f_P(z)}{1} \quad (2.31)$$

be given, where

$$f_P(z) = w_P + O(z + \xi). \quad (2.32)$$

The derivatives of (2.31) with respect to z

$$\left. \frac{d^0 f_1(z)}{dz^0} \right|_\xi, \left. \frac{d^0 f_1(z)}{dz^0} \right|_{x_k}, \left. \frac{d^1 f_1(z)}{dz^1} \right|_{x_k}, \dots, \left. \frac{d^{p_k-1} f_1(z)}{dz^{p_k-1}} \right|_{x_k}, \quad k = 1, 2, \dots, N \quad (2.33)$$

do not depend on the tail $f_P(z)$ satisfying (2.32).

Proof. By substituting the truncated power series of Stieltjes (2.1)-(2.2) to the recurrence relations (2.13) we obtain the formula (2.31) with the coefficients g_j , $j = 1, 2, \dots, P - 1$ uniquely depending on c_{mn} as follows (see (2.1)-(2.2))

$$\begin{aligned} g_1 &= \hat{g}_1(c_{01}); \quad g_2 = \hat{g}_2(c_{01}, c_{11}); \quad \dots, \quad g_{P_1} = \hat{g}_{P_1}(c_{01}, c_{11}, \dots, c_{(p_1-1)1}); \\ g_{P_1+1} &= \hat{g}_{P_1+1}(c_{01}, c_{11}, \dots, c_{(p_1-1)1}, c_{02}); \quad \dots \end{aligned} \quad (2.34)$$

and inversely

$$\begin{aligned} c_{01} &= \check{c}_{01}(g_1), \quad c_{11} = \check{c}_{11}(g_1, g_2); \quad \dots, \quad c_{(p_1-1)1} = \check{c}_{(p_1-1)1}(g_1, \dots, g_{P_1}); \\ c_{02} &= \check{c}_{02}(g_{11}, g_{21}, \dots, g_{P_1}, g_{P_1+1}); \quad \dots, \end{aligned} \quad (2.35)$$

where

$$c_{mn} = \frac{1}{m!} \left. \frac{d^m f_1(z)}{dz^m} \right|_{x_n}. \quad (2.36)$$

From (2.35) and (2.36), it results immediately, that (2.33) do not depend on $f_P(z)$ given by (2.32). ■

Theorem 2.9 *There is an one to one correspondence between the Stieltjes functions*

$$f_1 \in \Gamma_{x_1, x_2, \dots, x_N, \xi}^{p_1, p_2, \dots, p_N, 1} \quad \text{and} \quad f_P \in \Gamma_{\xi}^1 \quad (2.37)$$

satisfying the S -linear fractional transformation (2.26), where

$$\Gamma_{x_1, x_2, \dots, x_N, \xi}^{p_1, p_2, \dots, p_N, 1} = \left\{ f_1 ; f_1(z) = \int_0^{\infty} \frac{d\gamma_1(u)}{1+zu}, \quad f_1(z) \Big|_{x_1, x_2, \dots, x_N, \xi}^{p_1, p_2, \dots, p_N, 1}, \quad d\gamma_1(u) \geq 0 \right\} \quad (2.38)$$

and

$$\Gamma_{\xi}^1 = \left\{ f_P ; f_P(z) = \int_0^{\infty} \frac{d\gamma_P(u)}{1+zu}, \quad f(z) \Big|_{\xi}^1 = w_P + O(z - \xi), \quad d\gamma_P(u) \geq 0 \right\}. \quad (2.39)$$

Proof. Theorem 2.9 is a direct consequence of Theorems 1.16 and 2.8. ■

Now we state the last theorem presenting the properties of S -multipoint continued fractions to a Stieltjes function:

Theorem 2.10 *Assume that $(\alpha_1, \alpha_2, \dots, \alpha_N)$ and $(\beta_1, \beta_2, \dots, \beta_N)$ are two different permutations of natural numbers $(1, 2, \dots, N)$. Let the continued fraction expansions of $f_1(z)$*

$$f_1(z) = f_1 \left(z, \Big|_{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi}^{p_1, p_2, \dots, p_N, 1}, f_P^{\alpha}(z) \right) = f_1 \left(z, \Big|_{x_{\beta_1}, x_{\beta_2}, \dots, x_{\beta_N}, \xi}^{p_1, p_2, \dots, p_N, 1}, f_P^{\beta}(z) \right), \quad (2.40)$$

where

$$f_P^{\alpha}(\xi) = w_P^{\alpha}, \quad \text{and} \quad f_P^{\beta}(\xi) = w_P^{\beta}, \quad (2.41)$$

be given. For any permutations of $(\alpha_1, \alpha_2, \dots, \alpha_N)$ and $(\beta_1, \beta_2, \dots, \beta_N)$ the following identities

$$\begin{aligned} f_1 \left(z, \Big|_{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi}^{p_1, p_2, \dots, p_N, 1}, w_P^{\alpha} \right) &= f_1 \left(z, \Big|_{x_{\beta_1}, x_{\beta_2}, \dots, x_{\beta_N}, \xi}^{p_1, p_2, \dots, p_N, 1}, w_P^{\beta} \right) = [m_P/n_P](z), \\ [m_P/n_P](z) &= \frac{a_0 + a_1 z + \dots + a_{m_P} z^{m_P}}{1 + b_1 z + \dots + b_{n_P} z^{n_P}}, \\ m_P &= P - 1 - n_P, \quad n_P = E(P/2), \quad P = \sum_{j=1}^N p_j + 1; \end{aligned} \quad (2.42)$$

$$\text{if } P = 2k \text{ then } [m_P/n_P] = [k - 1/k];$$

$$\text{if } P = 2k + 1 \text{ then } [m_P/n_P] = [k/k]$$

are satisfied. Here $E(x)$ denotes the greatest integer not exceeding x .

Proof. The continued fraction expansions $f_1(z, \Big|_{x_{\alpha}}^p, f_P^{\alpha}(z))$ and $f_1(z, \Big|_{x_{\beta}}^p, f_P^{\beta}(z))$ are evaluated for the Stieltjes function $f_1(z)$, see (2.31). Hence the rational functions $f_1(z, \Big|_{x_{\alpha}}^p, w_P^{\alpha})$ and $f_1(z, \Big|_{x_{\beta}}^p, w_P^{\beta})$ are continued fractions to each other, cf. (2.40)-(2.41). On account of that the equations (2.42) are satisfied. ■

2.2 Fundamental inclusion relations for S -inclusion regions

In the sequel the Stieltjes functions $f_1(z)$ defined by

$$f_1(z) = \int_0^{1/\rho} \frac{d\gamma_1(u)}{1+zu}, \quad \Delta\gamma_1(0) = 0, \quad z \in \mathbb{C} \setminus [-\infty, -\rho], \quad \rho \geq 0 \quad (2.43)$$

will be investigated only. From the relation (2.43) and Theorem 2.6, it follows that $f_j(z)$, $j = 2, 3, \dots$ appearing in (2.13) are also Stieltjes functions

$$f_j(z) = \int_0^{1/\rho} \frac{d\gamma_j(u)}{1+zu}, \quad \rho \geq 0, \quad d\gamma_j(u) > 0, \quad j = 2, 3, \dots, \quad (2.44)$$

where the jumps of $\gamma_j(u)$ at $u = 0$ satisfy

$$\Delta\gamma_j(0) > 0 \text{ if } j \text{ is even and } \Delta\gamma_j(0) = 0 \text{ if } j \text{ is odd.} \quad (2.45)$$

Moreover, the coefficients of a continued fraction expansion (2.26) are positive, i.e. satisfy the inequalities

$$g_j > 0, \quad j = 1, 2, 3, \dots, P-1; \quad w_p > 0, \quad P = 1, 2, 3, \dots \quad (2.46)$$

The first order bounding function $F_{1,P}(z, u)$ is equal to (see Definition 1.21)

$$F_{1,P}(z, u) = w_P F_1(z - \xi, u), \quad F_1(z, u) = \begin{cases} (1+u) & \text{if } -1 \leq u \leq 0, \\ \frac{(1-u)}{1+(z-1)u} & \text{if } 0 \leq u \leq 1, \end{cases} \quad (2.47)$$

while the P -th order ones take the following forms (see(2.21))

$$\begin{aligned} F_{P,1}(z, u) &= \bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1+(z-x_k)} \times \frac{F_{1,P}(z, u)}{1} = \\ &= F_{P,1} \left(z, \begin{matrix} p_1, p_2, \dots, p_N, 1 \\ x_1, x_2, \dots, x_N, \xi \end{matrix}, F_{1,P}(z, u) \right) = \bigvee_{k=1}^N \mathbf{S}_{P_{k-1}+1}^{P_k} F_{1,P}(z, u) = \mathbf{S}_{P-1} F_{1,P}(z, u). \end{aligned} \quad (2.48)$$

Note that the formula (2.48) is obtained via replacing in (2.18) $f_P(z)$ by $F_{1,P}(z, u)$ and $f_1(z)$ by $F_{P,1}(z, u)$. Now we are in position to introduce the P -th order estimates of a Stieltjes function $f_1(z)$ as follows:

Definition 2.11 For a fixed $z \in \mathbb{C} \setminus [-\infty, -\rho]$ we call : 1)

$$\phi_{P,1}(z) = \{w \in \mathbb{C} : w = F_{P,1}(z, u) = \mathbf{S}_{P-1} F_{1,P}(z, u); \quad -1 \leq u \leq 1\}, \quad (2.49)$$

the P -th order complex boundary; 2)

$$\Phi_{P,1}(z) = \{w \in \mathbb{C} : w = \mathbf{S}_{P-1} \tau F_{1,P}(z, u); \quad 0 \leq \tau \leq 1, \quad -1 \leq u \leq 1\}, \quad (2.50)$$

the P -th order inclusion region; 3)

$$f_1(z) \in \Phi_{P,1}(z). \quad (2.51)$$

the P -th order inclusion relation.

Theorem 2.12 *The P – th order estimations of $f_1(z)$, i.e. $F_{P,1}(z, u)$ (2.48), $\phi_{P,1}(z)$ (2.49) and $\Phi_{P,1}(z)$ (2.50) evaluated from the truncated power expansions $f_1(z)_{x_1, x_2, \dots, x_N, \xi}^{p_1, p_2, \dots, p_N, 1}$ are the best.*

Proof. From $f_1(z)_{x_1, x_2, \dots, x_N, \xi}^{p_1, p_2, \dots, p_N, 1}$ it is not possible to find better estimations then (2.48), (2.49) and (2.50), since: (i) the correspondence between $F_{P,1}(z, u)$ (2.48) and $F_{1,P}(z, u)$ (2.47) is one-to-one, cf. Theorem 1.16; (ii) the bounding function $F_{1,P}(z, u)$ (2.47) is the best estimation of $f_P(z)$ for $f_P(\xi) = w_P$, cf. Theorem 1.22). ■

The recurrence S -algorithm (2.13)-(2.14), the S -relations (2.47)-(2.51) and Theorem 2.12 are the basic mathematical tools of the SMC FM.

2.2.1 Inclusion relations depending on P

Consider two contiguous bounding functions

$$F_{P-1,1}(z, u) = \mathbf{S}_{P_0+1}^{P_1} \mathbf{S}_{P_1+1}^{P_2} \mathbf{S}_{P_2+1}^{P_3} \dots \mathbf{S}_{P_{N-1}+1}^{P_N-1} F_{1,P-1}(z, u) \quad (2.52)$$

and

$$F_{P,1}(z, v) = \mathbf{S}_{P_0+1}^{P_1} \mathbf{S}_{P_1+1}^{P_2} \mathbf{S}_{P_2+1}^{P_3} \dots \mathbf{S}_{P_{N-1}+1}^{P_N-1} \mathbf{S}_{P_N}^{P_N} F_{1,P}(z, v) \quad (2.53)$$

satisfying the relations (cf. (2.2) and (2.16))

$$F_{P-1,1}(\xi, 0) = F_{P,1}(\xi, 0) = f_1(\xi) = \eta = w_1. \quad (2.54)$$

Our aim is to solve the equation

$$F_{P-1,1}(z, u) = F_{P,1}(z, v) \quad (2.55)$$

with respect to the real parameters $u \in [-1, +1]$ and $v \in [-1, +1]$. From (2.52) and (2.53), it follows

$$\mathbf{S}_{P_0+1}^{P_1} \mathbf{S}_{P_1+1}^{P_2} \mathbf{S}_{P_2+1}^{P_3} \dots \mathbf{S}_{P_{N-1}+1}^{P_N-1} F_{1,P-1}(z, u) = \mathbf{S}_{P_0+1}^{P_1} \mathbf{S}_{P_1+1}^{P_2} \dots \mathbf{S}_{P_{N-1}+1}^{P_N-1} \mathbf{S}_{P_N}^{P_N} F_{1,P}(z, v). \quad (2.56)$$

From the fact that the same operator

$$\mathbf{S}_{P_0+1}^{P_1} \mathbf{S}_{P_1+1}^{P_2} \mathbf{S}_{P_2+1}^{P_3} \dots \mathbf{S}_{P_{N-1}+1}^{P_N-1} \quad (2.57)$$

appears in both sides of (2.56), it follows that the solution of

$$F_{1,P-1}(z, u) = \mathbf{S}_{P_N}^{P_N} F_{1,P}(z, v), \quad F_{1,P-1}(\xi, 0) = \mathbf{S}_{P_N}^{P_N} F_{1,P}(\xi, 0) \quad (2.58)$$

solves the initial Eqs (2.54)-(2.56). The explicit form of (2.58)

$$F_{1,P-1}(z, u) = F_{2,P-1}(z, v), \quad F_{1,P-1}(\xi, 0) = F_{2,P-1}(\xi, 0) = w_{P-1} \quad (2.59)$$

takes the form of (1.181). On account of (1.184) and (1.185) we infer:

Conclusion 2.13 *For a fixed z the complex boundary $\phi_{P,1}(z)$*

$$\phi_{P,1}(z) = \{w \in \mathbb{C} : w = F_{P,1}(z, u); \quad -1 \leq u \leq 1\} \quad (2.60)$$

touches the complex one $\phi_{P-1,1}(z)$

$$\phi_{P-1,1}(z) = \{w \in \mathbb{C} : w = F_{P-1,1}(z, u); \quad -1 \leq u \leq 1\}$$

at the two points

$$F_{P,1}(z, -1) = F_{P,1}(z, 1) \text{ and } F_{P,1}(z, 0). \quad (2.61)$$

The regions $\Phi_{P,1}(z)$ and $\Phi_{P-1,1}(z)$ satisfy the fundamental inclusion relations

$$f_1(z) \in \Phi_{P,1}(z) \subset \Phi_{P-1,1}(z) \subset \dots \subset \Phi_{1,1}. \quad (2.62)$$

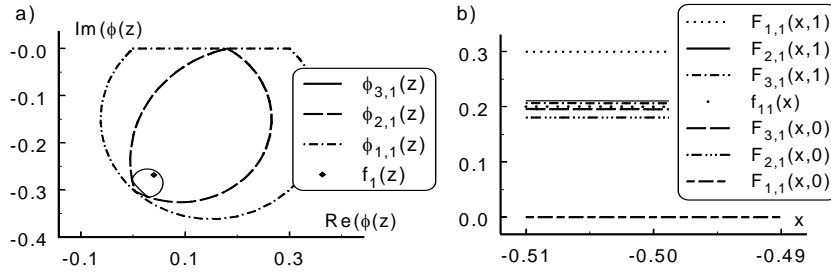


Fig. 2.2 The sequence of the first, second and third order boundaries from the truncated power expansions $f_1(z) = 0.3 + O(z + 2)$, $f_1(z) = 0.18 + O(z)$, $f_1(z) = 0.12 + O(z - 3)$ representing the Stieltjes function $f_1(z) = \frac{1}{z+2} \left(1 + \frac{1}{z+2} 2.5 \ln \frac{1+0.1(z+2)}{1+0.5(z+2)} \right)$. The complex boundaries $\phi_{1,1}(z)$, $\phi_{2,1}(z)$, $\phi_{3,1}(z)$ are computed for $z = -5 + i3$, while the real bounds $F_{1,1}(x, 0)$, $F_{1,1}(x, 1)$; $F_{1,2}(x, 0)$, $F_{1,2}(x, 1)$; $F_{1,3}(x, 0)$ and $F_{1,3}(x, 1)$ for $-0.51 \leq x \leq -0.49$.

For illustrating of (2.61) and (2.62) we consider the truncated power expansions

$$\begin{aligned} f_1(z)_0^1 &= 0.18073 + O(z); \quad f_1(z)_3^1 = 0.11527 + O(z - 3); \\ f_1(z)_\xi^1 &= w_1 + O(z - \xi), \quad \xi = -2, \quad w_1 = 0.30000 \end{aligned} \quad (2.63)$$

obtained from the Stieltjes function

$$f_1(z) = \frac{1}{z+2} \left(1 + \frac{2.5}{z+2} \ln \frac{1.2 + 0.1z}{2 + 0.5z} \right). \quad (2.64)$$

The results are depicted in Fig. 2.2.

First order estimation The first order bounding function $F_{1,1}(z, u)$ incorporating the power series $f_1(z)_{-2}^{+1}$ takes the form (cf. (2.63₂) and Definition 1.21)

$$F_{1,1}(z, u) = w_1 F_1(z + 2), \quad w_1 = f_1(-2) = 0.3. \quad (2.65)$$

Second order estimation From $f_1(z)_0^1$ and $f_1(z)_{-2}^{+1}$, it follows the second order bounding function $F_{2,1}(z, u)$ (cf. (2.63) and (2.48))

$$F_{2,1}(z, u) = \frac{g_1}{1 + z F_{1,2}(z, u)}, \quad F_{1,2}(z, u) = w_2 F_1(z + 2), \quad (2.66)$$

$$g_1 = 0.18073 \text{ and } w_2 = 0.19878. \quad (2.67)$$

Third order estimation The third order function $F_{3,1}(z, u)$ generated by $f_1(z)_0^1$, $f_1(z)_3^1$ and $f_1(z)_{-2}^{+1}$ is equal to (cf. (2.63) and (2.48))

$$F_{3,1}(z, u) = \frac{g_1}{1 + \frac{z g_2}{1 + (z - 3) F_{1,3}(z, u)}}, \quad F_{1,3}(z, u) = w_3 F_1(z + 2), \quad (2.68)$$

$$g_1 = 0.180733, \quad g_2 = 0.18930, \quad w_3 = 0.09529. \quad (2.69)$$

For both $z = -5 + i3$ and $z = x$, $-0.51 \leq x \leq -0.49$ the sequences of the estimates (2.65), (2.66) and (2.68) of a function (2.64) are computed and depicted in Fig. 2.2.

In the next two subsections the influence of ξ and η on estimates of a Stieltjes functions will be investigated. To this end we recall (2.4) and (2.48)

$$f_1^{\xi,\eta}(z) = f_1^{\xi,\eta}(z)_{\mathbf{p}}, \quad (\mathbf{p}) = \begin{pmatrix} p_1, p_2, \dots, p_N, 1 \\ x_1, x_2, \dots, x_N, \xi \end{pmatrix}, \quad f_1^{\xi,\eta}(\xi) = \eta \quad (2.70)$$

and

$$F_{P,1}^{\xi,\eta}(z, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)} \times \frac{F_{1,P}^{\xi,\eta}(z, u)}{1}, \quad (2.71)$$

$$F_{1,P}^{\xi,\eta}(z, u) = w_P^{\xi,\eta} F_1(z - \xi, u),$$

$$F_{P,1}^{\xi,\eta}(\xi, 0) = \eta.$$

Remark 2.14 *From the recurrence relations (2.13) we conclude that the coefficients g_j , $j = 1, 2, \dots, P - 1$ in (2.71) do not depend on ξ and η , while $w_P^{\xi,\eta}$ does depend.*

2.2.2 Inclusion relations depending on ξ

Consider two bounding functions $F_{P,1}^{\xi_1,\eta_1}(z, u)$ and $F_{P,1}^{\xi_2,\eta_1}$. From (2.70) and (2.71), it follows

$$F_{P,1}^{\xi_1,\eta_1}(\xi_1, 0) = F_{P,1}^{\xi_2,\eta_1}(\xi_2, 0) = \eta_1. \quad (2.72)$$

On account of Remark 2.14 the relations (2.71) and (2.72) lead to the inequalities

$$w_{P,1}(\xi_1, \eta_1) \leq w_{P,1}(\xi_2, \eta_1), \quad \text{if } \xi_1 \leq \xi_2, \quad (2.73)$$

while from Lemma 1.24, it follows

$$\Phi_1(z - \xi_1) \subset \Phi_1(z - \xi_2), \quad \text{if } \xi_1 \leq \xi_2. \quad (2.74)$$

Thus the relations (2.73) and (2.74) yield

$$\Phi_{1,P,1}^{\xi_1,\eta_1}(z) \subset \Phi_{1,P,1}^{\xi_2,\eta_1}(z), \quad \text{if } \xi_1 \leq \xi_2. \quad (2.75)$$

Conclusion 2.15 *For a fixed $z \in \mathbb{C} \setminus [-\infty, \xi_2]$, $P, 1$ and η_1 the inclusion relations*

$$f_1^{\xi_1,\eta_1}(z) \in \Phi_{P,1}^{\xi_1,\eta_1}(z, u) \subset \Phi_{P,1}^{\xi_2,\eta_1}(z, u) \quad (2.76)$$

are satisfied, provided that ξ_2 is not less than ξ_1

$$\xi_1 \leq \xi_2. \quad (2.77)$$

2.2.3 Inclusion relations depending on η

Now we deal with $F_{P,1}^{\xi_1,\eta_1}(z, u)$ and $F_{P,1}^{\xi_1,\eta_2}(z, u)$. From (2.70) and (2.71), it follows

$$F_{P,1}^{\xi_1,\eta_1}(\xi_1, 0) = \eta_1, \quad F_{P,1}^{\xi_2,\eta_2}(\xi_2, 0) = \eta_2. \quad (2.78)$$

As before the coefficients g_j do not depend on η , while $w_P^{\xi,\eta}$ does, cf. (2.71). Hence on account of (2.70) and (2.71) one can easily prove that

$$w_{P,1}^{\xi_1,\eta_1} \leq w_{P,1}^{\xi_1,\eta_2}, \quad \text{if } \eta_1 \leq \eta_2. \quad (2.79)$$

Conclusion 2.16 *For a fixed $P, 1$, ξ_1 and $z \in \mathbb{C} \setminus [-\infty, \xi_1]$ the inclusion relations*

$$f_1^{\xi_1,\eta_1}(z) \in \Phi_{P,1}^{\xi_1,\eta_1}(z) \subset \Phi_{P,1}^{\xi_1,\eta_2}(z) \quad (2.80)$$

are satisfied, provided that η_2 is not less than η_1

$$\eta_1 \leq \eta_2. \quad (2.81)$$

2.2.4 Inclusion relations depending on P, ξ, η

Assume now that $F_{P,1}^{\xi,\eta}(z, u)$ depends on the all parameters ξ, η and P . From (2.70) and (2.71), it follows

$$F_{P_I,1}^{\xi_1,\eta_1}(\xi_1, 0) = \eta_1, \quad F_{P_{II},1}^{\xi_2,\eta_2}(\xi, 0) = \eta_2. \quad (2.82)$$

Theorem 2.17 For $z \in \mathbb{C} \setminus [-\infty, \xi_2]$ and $j = 1, 2, \dots, N$ the S -inclusion regions $\Phi_{P_I,1}^{\xi_1,\eta_1}(z)$ and $\Phi_{P_{II},1}^{\xi_2,\eta_2}(z)$ constructed from the non-decreasing truncated Stieltjes series (cf. Definition (2.4))

$$f_1^{\xi_1,\eta_1}(z) = \eta_1 + O(z - \xi_1), \quad f_1^{\xi_1,\eta_1} = \sum_{i=0}^{p_j^I} c_{ij}(z - x_j)^i + O((z - x_j)^{p_j}), \quad (2.83)$$

$$f_1^{\xi_2,\eta_2}(z) = \eta_2 + O(z - \xi_2), \quad f_1^{\xi_2,\eta_2}(z) = \sum_{i=0}^{p_j^{II}} c_{ij}(z - x_j)^i + O((z - x_j)^{p_j})$$

obey the following relations

$$f_1^{\xi_1,\eta_1}(z) \in \Phi_{P_I,1}^{\xi_1,\eta_1}(z) \subset \Phi_{P_{II},1}^{\xi_2,\eta_2}(z), \quad (2.84)$$

provided the inequalities

$$\eta_1 \leq \eta_2, \quad \xi_1 \leq \xi_2, \quad P_{II} \leq P_I \quad (2.85)$$

are satisfied.

Proof. The inclusion relations (2.84) are the direct consequence of the Conclusions (2.13), (2.15) and (2.16). ■

The inclusion relations (2.84)-(2.85) have a consequence that the S -multipoint inclusion region $\Phi_{P,1}^{\xi,\eta}(z)$ is the optimal estimate of $f_1^{\xi,\eta}(z)$ obtainable from the given number of coefficients (P is fixed) and that the use of additional coefficients (higher P) improves $\Phi_{P,1}^{\xi,\eta}(z)$.

Theorems 2.12 and 2.17 are fundamental, for they provide the best estimates of a Stieltjes function $f_1(z)$ from the truncated power series expanded at an number of real points. It is worth noting that the substitution of

$$x_1 = 0, \quad \xi_1 = \xi_2 = -R, \quad \eta_1 = \eta_2 = \infty, \quad p_2 = p_3 = \dots = p_N = 0 \quad (2.86)$$

to the relations (2.83)-(2.85) reduces the Theorem 2.17 to the Theorem 17.1 proved by Baker [6, Theorem 17.1].

2.3 General S -estimates of a complex Stieltjes functions

Now we are able to investigate the basic problem of an approximation of a Stieltjes function $f_1(z)$ stated as follows:

Problem 2.18 By starting from N truncated power expansions

$$f_1(z) = f_1(z)_{\mathbf{x}}^{\mathbf{p}}, \quad \left(\begin{matrix} \mathbf{p} \\ \mathbf{x} \end{matrix} \right) = \left(\begin{matrix} p_1, p_2, \dots, p_N, 1 \\ x_1, x_2, \dots, x_N, \xi \end{matrix} \right) \quad (2.87)$$

we find the best bounding function $F_{P,1}(z, u)$ estimating $f_1(z)$.

To solve the Problem 2.18 the parametric power series $f_1^{\xi,\eta}(z)_x^{\mathbf{p}}$ associated with $f_1(z)_x^{\mathbf{p}}$ is needed

$$f_1^{\xi,\eta}(z) = f_1^{\xi,\eta}(z)_x^{\mathbf{p}}, \quad (\mathbf{p}) = \begin{pmatrix} p_1, p_2, \dots, p_N, 1 \\ x_1, x_2, \dots, x_N, \xi \end{pmatrix}, \quad f_1(\xi) = \eta. \quad (2.88)$$

The continued fraction expansion of $f_1^{\xi,\eta}(z)$ computed from (2.88) takes the form (see (2.21))

$$f_1^{\xi,\eta}(z) = \mathbf{S}_{P-1}^{(z)} f_P^{\xi,\eta}(z), \quad \text{where } f_P^{\xi,\eta}(\xi) = w_P^{\xi,\eta} \text{ and } \eta = \mathbf{S}_{P-1}^{(z)} f_P^{\xi,\eta}(\xi). \quad (2.89)$$

Formula (2.89) leads to the bounding function $F_{P,1}(z, u)$ (cf. (2.71) and (2.89))

$$F_{P,1}(z, u) = \bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)} \times \frac{w_P^{\xi,\eta} F_1(z - \xi, u)}{1}, \quad (2.90)$$

$$w_P^{\xi,\eta} = (\mathbf{S}_{P-1}^{(\xi)})^{-1} \eta.$$

Finally from (2.84), (2.85), (2.90), (2.88) and (2.87), it follows the solution $F_{P,1}(z, u)$ of the Problem 2.18

$$\begin{aligned} F_{P,1}(z, u) &= \lim_{\xi \rightarrow x} \lim_{\eta \rightarrow \infty} \bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)} \times \frac{w_P^{\xi,\eta} F_1(z - \xi, u)}{1} = \\ &= \lim_{\xi \rightarrow x} \bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)} \times \frac{w_P^{\xi,\infty} F_1(z - x, u)}{1}, \end{aligned} \quad (2.91)$$

$$w_P^{\xi,\infty} = \lim_{\eta \rightarrow \infty} ((\mathbf{S}_{P-1}^{(\xi)})^{-1} \eta),$$

where (see (2.89))

$$x = \min(x_j, j = 1, 2, \dots, N). \quad (2.92)$$

2.4 Particular S-estimates of a complex Stieltjes functions

In this section a few particular cases of the general bounding functions $F_{P,1}(z, u)$ (2.91)-(2.92) will be investigated.

2.4.1 Stieltjes function expanded at zero

(a) The first term is available only Consider the truncated power expansion $f_1(z)_x^{\mathbf{p}}$ of $f_1(z)$ given by

$$f_1(z) = f_1(z)_x^{\mathbf{p}}, \quad (\mathbf{p}) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (2.93)$$

The parametric series $f_1^{\xi,\eta}(z)_x^{\mathbf{p}}$ accompanying (2.93) take the forms (see Theorem (2.17))

$$f_1^{\xi,\eta}(z)_x^{\mathbf{p}}, \quad (\mathbf{p}) = \begin{pmatrix} 1, 1 \\ 0, \xi \end{pmatrix} \quad (2.94)$$

or explicitly

$$f_1^{\xi,\eta}(z) = \eta + O(z - \xi), \quad f_1^{\xi,\eta}(z) = g_1 + O(z), \quad \xi < 0, \quad g_1 < \eta. \quad (2.95)$$

For (2.95) the general formula (2.71) reduces to

$$F_{2,1}(z, u) = \lim_{\xi \rightarrow x} \frac{g_1}{1 + (z - x) w_P^{\xi,\infty} F_1(z - \xi, u)}, \quad w_P^{\xi,\infty} = \lim_{\eta \rightarrow \infty} \frac{g_1 - \eta}{\eta \xi} = \frac{1}{-\xi}, \quad x = 0. \quad (2.96)$$

Relations (2.96) yield

$$F_{2,1}(z, u) = \lim_{\xi \rightarrow 0} \left(\frac{g_1}{1 + \frac{z}{-\xi} F_1(z, u)} \right) = g_1 F_2(z, \tau), \quad (2.97)$$

where

$$F_2(z, u) = \begin{cases} \frac{-\tau}{1 + (z-1)(1+\tau)} & \text{if } -1 \leq \tau \leq 0, \\ \tau & \text{if } 0 \leq \tau \leq 1. \end{cases} \quad (2.98)$$

For an increasing values of r the convergence of $1/(1+zrF_1(z, u))$ to $F_2(z, u)$, $-1 \leq u \leq 1$ is illustrated in Fig. 2.3, cf. (2.97) and (2.98). It can be easily checked that $F_2(z, u)$ coincides with the elementary bounding function $F_1(z, u)$ (1.154)

$$F_2(z, \tau) = F_1(z, u), \quad -1 \leq u, \tau \leq 1. \quad (2.99)$$

From (2.97) and (2.98) the identity follows

$$\lim_{r \rightarrow \infty} \left(\frac{1}{1 + (z-x)rF_1(z-x, u)} \right) = F_2(z-x, \tau). \quad (2.100)$$

The relation (2.100) will be used to simplify the last terms of the S -continued fraction expansions of $f_1(z)$.

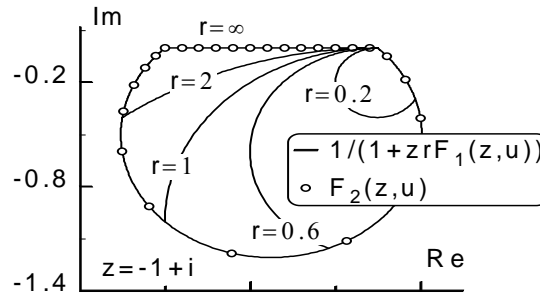


Fig. 2.3 The sequence of $(1 + zrF_1(z, u))^{-1}$, $r = -1/\xi$, $z = -1 + i$ converging to the bounding function $F_2(z, u)$, cf. (2.98).

2.4.2 Stieltjes function expanded at a number of real points

(b) **The case $\xi < x_N = \min(x_j, j = 1, 2, \dots, N)$** Now we are prepared to explore in detail the bounding function (2.91) constructed from

$$f_1(z)_x^p, \quad \binom{p}{x} = \binom{p_1, p_2, \dots, p_N}{x_1, x_2, \dots, x_N} \quad (2.101)$$

The parametric series $f_1^{\xi, \eta}(z)_x^p$ associated with $f_1(z)_x^p$ (2.101) take the forms

$$f_1^{-\xi, \eta}(z)_x^p, \quad \binom{p}{x} = \binom{p_1, p_2, \dots, p_N, 1}{x_1, x_2, \dots, x_N, \xi}. \quad (2.102)$$

From (2.91)-(2.92) and (2.102) we obtain

$$w_P^{\xi, \infty} = \lim_{\eta \rightarrow \infty} ((\mathbf{S}_{P-1}^{(\xi)})^{-1} \eta), \quad x = x_N, \quad (2.103)$$

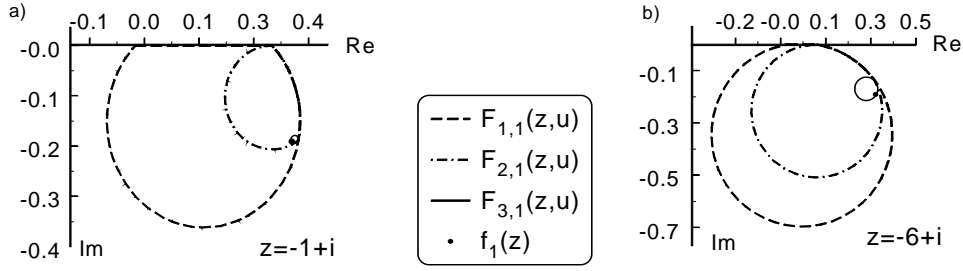


Fig. 2.4 The lens-shaped bounding functions $F_{P,1}(z, u)$ $P = 1, 2, 3$ evaluated from the truncated power series $f_1(z)_0^3 = 0.30 - 0.103z + 0.039z^2 + O(z^3)$, where $f_1(z) = \frac{1}{z} \left(1 + \frac{2.5}{z} \ln \frac{(1+0.1z)}{(1+0.5z)} \right)$.

$$F_{P,1}(z, u) = \lim_{\xi \rightarrow x_N} \left(\prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k) \times \frac{w_P^{\xi, \infty} F_1(z - x_N, u)}{1}} \right), \quad (2.104)$$

or more precisely

$$\prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k-1} \frac{g_j}{1 + (\xi - x_k) \times \frac{g_{P_N}}{1 + (\xi - x_N) w_P^{\xi, \infty}}} = \infty, \quad (2.105)$$

$$F_{P,1}(z, u) = \lim_{\xi \rightarrow x_N} \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k-1} \frac{g_j}{1 + (z - x_k) \times \frac{g_{P_N}}{1 + (z - x_N) F_1(z - x_N, u) w_P^{\xi, \infty}}}. \quad (2.106)$$

Since $\lim_{\xi \rightarrow x_N} \frac{(\xi - x_N) g_{P_N}}{1 + (\xi - x_N) w_P^{\xi, \infty}} \neq 0$ the relation (2.105) yields

$$w_P^{\xi, \infty} = -\frac{1}{\xi - x_N} + C + O(\xi - x_N), \quad C < \infty, \quad \xi < x_N. \quad (2.107)$$

From (2.100), (2.106) and (2.107), it follows

$$F_{P,1}(z, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k - \delta_{kN}} \frac{g_j}{1 + (z - x_k) \times \frac{g_{P-1} F_2(z - x_N, u)}{1}}. \quad (2.108)$$

As an example illustrating (2.108) let us consider the truncated power expansion

$$f_1(z)_0^3 = 0.30 - 0.10333z + 0.039z^2 + O(z^3) \quad (2.109)$$

obtained from the Stieltjes function

$$f_1(z) = \frac{1}{z} \left(1 + \frac{2.5}{z} \ln \frac{1 + 0.1z}{1 + 0.5z} \right). \quad (2.110)$$

The sequence of the first, second and third order bounding functions $F_{p,1}(z, u)$, $p = 1, 2, 3$ evaluated from (2.109) takes the form

$$F_{1,1}(z, u) = g_1 F_2(z, u); \quad F_{2,1}(z, u) = \frac{g_1}{1 + z} \times \frac{g_2 F_2(z, u)}{1}; \quad (2.111)$$

$$F_{3,1}(z, u) = \frac{g_1}{1 + z} \times \frac{g_2}{1 + z} \times \frac{g_3 F_2(z, u)}{1}; \quad g_1 = 0.3, \quad g_2 = 0.3444, \quad g_3 = 0.033.$$

The results (2.111) estimating (2.110) are shown in Fig. 2.4.

(c) **The case $\xi < \mathbf{x}_1 = \min(\mathbf{x}_j, j = 1, 2, \dots, N)$** The parametric expansions $f_1^{\xi, \eta}(z)_x^p$ associated with (2.101) are equal to (2.102). From (2.91)-(2.92) one obtains

$$w_P^{x_1, \infty} = \lim_{\xi \rightarrow x_1} \lim_{\eta \rightarrow \infty} ((\mathbf{S}_{P-1}^{(\xi)})^{-1} \eta), \quad x = x_1, \quad (2.112)$$

$$F_{P,1}(z, u) = \bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)} \times \frac{w_P^{x_1, \infty} F_1(z - x_1, u)}{1}. \quad (2.113)$$

(d) **The cases $\xi < \mathbf{x}_N = \min(\mathbf{x}_j, j = 1, 2, \dots, N-1)$ and $\xi < \mathbf{x}_1 = \min(\mathbf{x}_j, j = 2, 3, \dots, N)$** Let's focus our attention on the bounding functions $F_{P,1}^{x_N, \infty}(z, u)$ (2.108) and $F_{P,1}^{x_1, \infty}(z, \tau)$ (2.113) given by

$$F_{P,1}^{x_1, \infty}(z, u) = \bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \frac{g_j^{x_1}}{1 + (z - x_k)} \times \frac{w_P(x_1, \infty) F_1(z - x_1, u)}{1}, \quad (2.114)$$

$$F_{P-1,1}^{x_N, \infty}(z, \tau) = \bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k - \delta_{kN}} \frac{g_j^{x_N}}{1 + (z - x_k)} \times \frac{g_{P-1}^{x_N} F_2(z - x_N, \tau)}{1}.$$

It is proved in the sequel (see Theorem 2.21) that even though the coefficients $g_j^{x_1}$ and $g_j^{x_N}$ are different the bounding functions (2.114₁) and (2.114₂) generate identical complex boundaries, i.e.

$$\begin{aligned} \psi_{P,1}^{x_1, \infty}(z) &= \{w \in \mathbb{C} : w = F_{P,1}^{x_1, \infty}(z, u); -1 \leq u \leq 1\}, \\ \psi_{P,1}^{x_N, \infty}(z) &= \{w \in \mathbb{C} : w = F_{P,1}^{x_N, \infty}(z, \tau); -1 \leq \tau \leq 1\}. \end{aligned} \quad (2.115)$$

As an example we consider the truncated power expansions of $f_1(z)$ given by

$$f_1(z)_{x_1}^1 = 1 + O(z - x_1) \text{ and } f_1(z)_{x_2}^1 = \frac{1}{7} + O(z - x_2), \quad x_1 = 0, \quad x_2 = 3, \quad (2.116)$$

or by

$$f_1(z)_{x_1}^1 = \frac{1}{7} + O(z - x_1) \text{ and } f_1(z)_{x_2}^1 = 1 + O(z - x_2), \quad x_1 = 3, \quad x_2 = 0. \quad (2.117)$$

The relations (2.114₁) and (2.114₂) evaluated from (2.116) and (2.117) take the forms

$$F_{3,1}^{x_1, \infty}(z, u) = \frac{1}{1 + \frac{2z}{1 + \frac{1}{3}(z-3)F_1(z, u)}} \text{ and } F_{3,1}^{x_2, \infty}(z, \tau) = \frac{\frac{1}{7}}{1 + \frac{2}{7}(z-3)F_2(z, \tau)}. \quad (2.118)$$

In spite of the different structures of the bounding functions $F_{3,1}^{x_1, \infty}(z, u)$ and $F_{3,1}^{x_2, \infty}(z, \tau)$ the complex boundaries $\phi_{3,1}^{x_1, \infty}(z)$ and $\phi_{3,1}^{x_2, \infty}(z)$ coincide, see Fig. 2.5.

2.5 Diagonal and overdiagonal multipoint Padé approximants

2.5.1 Definitions

Let us define the diagonal and overdiagonal multipoint Padé approximants to an analytical function $f_1(z)$ expanded at real points $x_1, x_2, \dots, x_N, x_{N+1}$, where $\max(x_1, x_2, \dots, x_N, x_{N+1}) < \infty$.

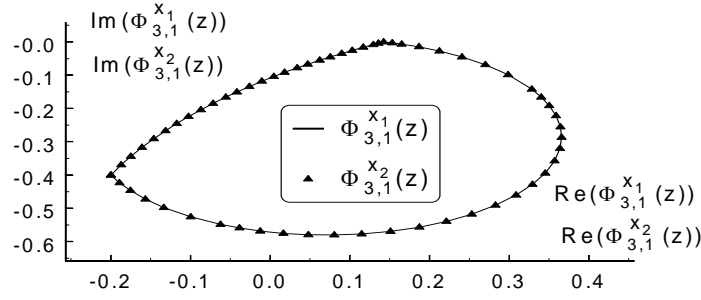


Fig. 2.5 The complex boundaries $\phi_{3,1}^{x_1,\infty}(z, u)$ and $\phi_{3,1}^{x_2,\infty}(z, \tau)$ generated by the bounding functions $F_{3,1}^{x_1,\infty}(z, u)$ and $F_{3,1}^{x_2,\infty}(z, \tau)$. They coincide, cf. (2.118).

Definition 2.19 Let $\mathbf{p} = (p_1, p_2, \dots, p_N, p_{N+1})$ denote the numbers of coefficients of the power expansion of $[m_P/n_P](z)$ at points $\mathbf{x} = (x_1, x_2, \dots, x_N, x_{N+1})$, respectively, while $E(y)$ is the greatest integer not exceeding y . The rational function

$$[m_P/n_P](z) = [m_P/n_P]_{\mathbf{x}}^{\mathbf{p}}(z), \quad \left(\begin{smallmatrix} \mathbf{p} \\ \mathbf{x} \end{smallmatrix}\right) = \begin{pmatrix} p_1, p_2, \dots, p_N, p_{N+1} \\ x_1, x_2, \dots, x_N, x_{N+1} \end{pmatrix}, \quad (2.119)$$

where

$$[m_P/n_P]_{\mathbf{x}}^{\mathbf{p}}(z) = \frac{a_0 + a_1 z^1 + a_2 z^2 + \dots + a_{m_P} z^{m_P}}{1 + b_1 z^1 + b_2 z^2 + \dots + b_{n_P} z^{n_P}}, \quad (2.120)$$

$$m_P = P - 1 - n_P, \quad n_P = E(P/2), \quad P = \sum_{j=1}^{N+1} p_j,$$

we call the diagonal ($m_P = n_P$) and overdiagonal ($m_P = n_P - 1$) multipoint Padé approximant to power series $f_1(z)$, if

$$f_1(z) - [m_P/n_P](z) = O((z - x_j)^{p_j}), \quad j = 1, 2, \dots, N, N+1 \text{ as } z \rightarrow x_j. \quad (2.121)$$

By way of illustration of Definition 2.19 the multipoint Padé approximants $[m_P/n_P]_{\mathbf{x}}^{\mathbf{p}}(z)$ to the truncated power expansions $\exp(z)_{\mathbf{x}}^{\mathbf{p}}$ of $\exp(z)$

$$\exp(z) = \exp(z)_{\mathbf{x}}^{\mathbf{p}}, \quad \left(\begin{smallmatrix} \mathbf{p} \\ \mathbf{x} \end{smallmatrix}\right) = \begin{pmatrix} 2, 1, +1 \\ 0, 1, -1 \end{pmatrix} \quad (2.122)$$

will be constructed. From (2.122), it follows that

$$P = 4, \quad n_4 = 2, \quad m_4 = 1. \quad (2.123)$$

On account of (2.123) the formula (2.119) reduces to

$$[m_4/n_4](z) = [1/2](z) = [1/2]_{0,1,-1}^{2,1,+1}(z) = \frac{a_0 + a_1 z^1}{1 + b_1 z^1 + b_2 z^2}. \quad (2.124)$$

By substituting (2.122) and (2.124) into (2.121) one obtains

$$\begin{aligned} \exp(z) - [1/2]_{0,1,-1}^{2,1,+1}(z) &= (1 - a_0) + (1 - a_1 + a_0 b_1)z = O(z^2), \\ \exp(z) - [1/2]_{0,1,-1}^{2,1,+1}(z) &= \left(2.718 - \frac{a_0 + a_1}{1 + b_1 + b_2}\right) = O((z - 1)^1), \\ \exp(z) - [1/2]_{0,1,-1}^{2,1,+1}(z) &= \left(0.368 - \frac{a_0 - a_1}{1 - b_1 + b_2}\right) = O((z + 1)^1). \end{aligned} \quad (2.125)$$

Hence

$$a_0 = 1, \quad \frac{a_0 - a_1}{1 - b_1 + b_2} = 0.368, \quad a_1 - a_0 b_1 = 1, \quad \frac{a_0 + a_1}{1 + b_1 + b_2} = 2.718 \quad (2.126)$$

and finally (2.124)-(2.126) yield

$$[1/2](z) = [1/2]_{0,1,-1}^{2,1,+1}(z) = \frac{1 + 0.3227z}{1 - 0.6774z + 0.1640z^2}. \quad (2.127)$$

It is worth noting that on the basis of (cf. (2.119)-(2.121)) we have

$$[1/2]_{0,1,-1}^{2,1,+1}(z) = [1/2]_{1,0,-1}^{1,2,+1}(z) = [1/2]_{1,-1,0}^{1,+1,2}(z) = [1/2]_{-1,0,1}^{+1,2,1}(z). \quad (2.128)$$

Now we prove the following corollary interrelating the bounding functions $F_{P,1}(z, u)$, $u = -1, 0, 1$ with the multipoint Padé approximants $[m_P/n_P](z)$ and $[m_{P-1}/n_{P-1}](z)$.

Corollary 2.20 *The values of bounding functions $F_{P,1}(z, u)$, $u = -1, 0, 1$ (cf. (2.20) and (2.90))*

$$F_{P,1}(z, 0) = \bigvee_{k=1}^N \mathbf{S}_{P_{k-1}+1}^{P_k} F_{1,P}(z, 0), \quad F_{1,P}(z, 0) = w_P,$$

$$F_{P,1}(z, -1) = \bigvee_{k=1}^N \mathbf{S}_{P_{k-1}+1}^{P_k} F_{1,P}(z, -1) = F_{P,1}(z, 1) = \bigvee_{k=1}^N \mathbf{S}_{P_{k-1}+1}^{P_k} F_{1,P}(z, 1), \quad (2.129)$$

$$F_{1,P}(z, -1) = F_{1,P}(z, 1) = 0$$

and the multipoint Padé approximants

$$[m_P/n_P]_{\mathbf{x}}^{p(P)}(z), \quad \begin{pmatrix} p(P) \\ \mathbf{x} \end{pmatrix} = \begin{pmatrix} p_1, p_2, \dots, p_N, 1 \\ x_1, x_2, \dots, x_N, \xi \end{pmatrix}, \quad (2.130)$$

$$[m_{P-1}/n_{P-1}]_{\mathbf{x}}^{p(P-1)}(z), \quad \begin{pmatrix} p(P-1) \\ \mathbf{x} \end{pmatrix} = \begin{pmatrix} p_1, p_2, \dots, p_N, 0 \\ x_1, x_2, \dots, x_N, \xi \end{pmatrix}$$

coincide, i.e.

$$F_{P,1}(z, 1) = [m_{P-1}/n_{P-1}]_{\mathbf{x}}^{p(P-1)}(z) = F_{P,1}(z, -1), \quad (2.131)$$

$$F_{P,1}(z, 0) = [m_P/n_P]_{\mathbf{x}}^{p(P)}(z).$$

Proof. From Definition 2.19 and Theorem 2.8, it follows the identities (2.131) immediately. ■

To illustrate the Corollary (2.20) we use the bounding function

$$F_{3,1}(z, u) = \frac{1}{1 - \frac{0.632z}{1 + (z-1)F_{1,3}(z, u)}}, \quad F_{1,3}(z, 0) = w_3 = 0.316, \quad F_{1,3}(z, 1) = 0 \quad (2.132)$$

constructed from the input data

$$\exp(z) = \exp(z)_{\mathbf{x}}^{\mathbf{p}}, \quad \begin{pmatrix} \mathbf{p} \\ \mathbf{x} \end{pmatrix} = \begin{pmatrix} 1, 1, +1 \\ 0, 1, -1 \end{pmatrix}. \quad (2.133)$$

By substituting (2.132₃) and (2.132₃) into (2.132₁) we obtain the relations

$$F_{3,1}(z, 0) = \frac{1}{1 - \frac{0.632z}{1 + 0.316(z-1)}} = \frac{1 + 0.462z}{1 - 0.462z} = [1/1]_{0,1,-1}^{1,1,+1}(z), \quad (2.134)$$

$$F_{3,1}(z, 1) = \frac{1}{1 - 0.632z} = [0/1]_{0,1}^{1,1}(z)$$

confirming the equalities (2.131). Note that the function $\exp(z)$ is not a Stieltjes one, cf. 2.133.

2.5.2 The complex boundaries as parametric multipoint Padé approximants

Consider the following two parametric functions

$$F_{P,1}(z, u), \quad u \in [-1, 0]; \quad F_{P,1}(z, u), \quad u \in [0, 1] \quad (2.135)$$

and

$$F_{P+1,1}(z, u), \quad u \in [-1, 0]; \quad F_{P+1,1}(z, u), \quad u \in [0, 1] \quad (2.136)$$

forming the bounding ones

$$F_{P,1}(z, u), \quad u \in [-1, 1]; \quad F_{P+1,1}(z, u), \quad u \in [-1, 1], \quad (2.137)$$

where we have

$$F_{P,1}(z, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)} \times \frac{F_{1,P}(z, u)}{1}, \quad (2.138)$$

$$F_{1,P}(z, u) = w_P F_1(z - \xi, u),$$

$$F_{P+1,1}(z, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)} \times \frac{g_P}{1 + (z - x_N) F_{1,P+1}(z, u)}, \quad (2.139)$$

$$F_{1,P+1}(z, u) = w_{P+1} F_1(z - \xi, u)$$

and

$$F_{1,P}(z, -1) = F_{1,P}(z, 1) = F_{1,P+1}(z, -1) = F_{1,P+1}(z, 1) = 0, \quad (2.140)$$

$$F_{1,P}(z, 0) = w_P, \quad F_{1,P+1}(z, 0) = w_{P+1}.$$

Since

$$F_{P+1,1}(\xi, 0) = F_{P,1}(\xi, 0) \quad (2.141)$$

then

$$F_{1,P}(\xi, 0) = \frac{g_P}{1 + (\xi - x_N) F_{1,P+1}(\xi, 0)}. \quad (2.142)$$

From (2.140)-(2.142), it follows

$$w_{P+1}(g_P) = \frac{g_P - w_P}{w_P(\xi - x_N)}. \quad (2.143)$$

According to Conclusion 2.13 the next curve (2.137₂) touches the previous one (2.137₁) at two points $F_{P+1,1}(z, 1)$ and $F_{P+1,1}(z, 0)$. On account of that the parametric multipoint Padé approximants $H_{P+1,1}(z, g_P)$

$$H_{P+1,1}(z, g_P) = \begin{cases} F_{P+1,1}(z, 1, -g_P) & \text{if } -w_P \leq g_P \leq 0, \\ F_{P+1,1}(z, 0, g_P) & \text{if } 0 \leq g_P \leq w_P \end{cases} \quad (2.144)$$

depending on the coefficient g_P , where (cf. (2.138), (2.139) and (2.143))

$$F_{P+1,1}(z, 1, -g_P) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)} \times \frac{-g_P}{1}, \quad (2.145)$$

$$F_{P+1,1}(z, 0, g_P) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)} \times \frac{g_P}{1 + (z - x_N) \frac{g_P - w_P}{w_P(\xi - x_N)}}$$

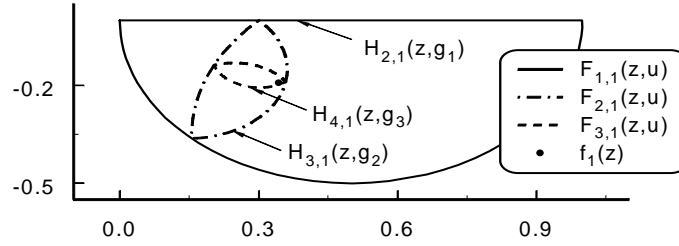


Fig. 2.6 The bounding functions $F_{p,1}(z, u)$, $-1 \leq u \leq 1$ and $H_{p+1,1}(z, g_p)$, $-w_P \leq g_P \leq w_P$, $p = 1, 2, 3$ from the Stieltjes series $f_1(z)_0^3 = 0.3 - 0.1034z + 0.039z^2 + O(z^3)$, $f_1(z)_{-1}^{+1} = \eta + O(z+1)$, where $z = -1 + i$.

coincide with (2.135₁) and (2.135₂), respectively, i.e.

$$\begin{aligned} \chi_{P+1,1}(z) &= \phi_{P,1}(z), \\ \chi_{P+1,1}(z) &= \{w \in \mathbb{C} : w = H_{P+1,1}(z, g_P); g_P \in [-w_P, w_P]\}, \\ \phi_{P,1}(z) &= \{w \in \mathbb{C} : w = F_{P,1}(z, u); u \in [-1, 1]\}. \end{aligned} \quad (2.146)$$

As an example illustrating the relations (2.146) we consider the truncated power series

$$\begin{aligned} f_1(z)_0^3 &= 0.3 - 0.1034z + 0.0390z^2 + O(z^3), \\ f_1(z)_{-1}^{+1} &= f_1(-1) + O(z+1), \quad f_1(-1) = 0.469 \end{aligned} \quad (2.147)$$

evaluated from the Stieltjes function

$$f_1(z) = \frac{1}{z} \left(1 + \frac{2.5}{z} \ln \frac{1 + 0.1z}{1 + 0.5z} \right). \quad (2.148)$$

The parametric multipoint Padé approximants (2.145) to the truncated power series (2.147) are of the form

$$\begin{aligned} F_{1,1}(z, 1) &= 0, \quad F_{1,1}(z, 0) = 1, \quad F_{2,1}(z, 1, g_1) = g_1, \quad F_{2,1}(z, 0, g_1) = \frac{g_1}{1 + (1 - g_1)z}, \\ F_{3,1}(z, 1, g_2) &= \frac{0.30}{1 + g_2z}, \quad F_{3,1}(z, 0, g_2) = \frac{0.30}{1 + \frac{g_2z}{1 + \frac{0.7 - g_2}{0.7}z}}, \\ F_{4,1}(z, 1, g_3) &= \frac{0.30}{1 + \frac{0.345z}{1 + g_3z}}, \quad F_{4,1}(z, 0, g_3) = \frac{0.30}{1 + \frac{0.345z}{1 + \frac{g_3z}{1 + \frac{0.508 - g_3}{0.508}z}}}, \end{aligned} \quad (2.149)$$

where

$$0 \leq g_1 \leq 1, \quad 0 \leq g_2 \leq 0.7, \quad 0 \leq g_3 \leq 0.508. \quad (2.150)$$

For $z = -1 + i$ the values of bounding (2.149) and Stieltjes (2.148) functions are evaluated and shown in Fig. 2.6.

Now we prove theorem exploiting the different continued fraction structures of the S -estimates of a Stieltjes function $f_1(z)$.

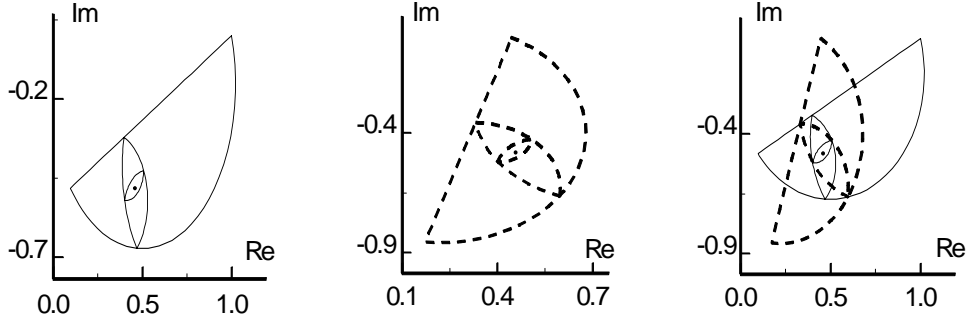


Fig. 2.7 The best bounding functions $F_{2,1} \left(\begin{smallmatrix} 1,+1 \\ 4,-1 \end{smallmatrix}, z, u \right)$, $F_{3,1} \left(\begin{smallmatrix} 1,1,+1 \\ 4,9,-1 \end{smallmatrix}, z, u \right)$, $F_{4,1} \left(\begin{smallmatrix} 1,1,1,+1 \\ 4,9,19,-1 \end{smallmatrix}, z, u \right)$, $F_{2,1} \left(\begin{smallmatrix} 1,+1 \\ 19,-1 \end{smallmatrix}, z, u \right)$, $F_{3,1} \left(\begin{smallmatrix} 1,1,+1 \\ 19,4,-1 \end{smallmatrix}, z, u \right)$, $F_{4,1} \left(\begin{smallmatrix} 1,1,1,+1 \\ 19,4,9,-1 \end{smallmatrix}, z, u \right)$ from the input data (2.157), $z = 1 + i10$.

Theorem 2.21 Let $F_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_1, x_2, \dots, x_N, \xi \end{smallmatrix}, u \right)$ be the bounding function constructed from the truncated power series of Stieltjes $f_1(z)_{x_1, x_2, \dots, x_N, \xi}^{p_1, p_2, \dots, p_N, 1}$. For all permutations $(\alpha_1, \alpha_2, \dots, \alpha_N)$ of natural numbers $(1, 2, \dots, N)$ the complex boundaries

$$\phi_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_1, x_2, \dots, x_N, \xi \end{smallmatrix} \right) \text{ and } \phi_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi \end{smallmatrix} \right) \quad (2.151)$$

generated by the bounding functions

$$F_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_1, x_2, \dots, x_N, \xi \end{smallmatrix}, u \right) \text{ and } F_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi \end{smallmatrix}, u \right) \quad (2.152)$$

coincide (cf. (2.49))

$$\phi_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_1, x_2, \dots, x_N, \xi \end{smallmatrix} \right) = \phi_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi \end{smallmatrix} \right). \quad (2.153)$$

Proof. For a fixed permutation of $(\alpha_1, \alpha_2, \dots, \alpha_N)$ the two arcs of circles generated by $F_{P,1}(z, u)$ are determined uniquely by the two sets of three points

$$\left| \begin{array}{l} F_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi \end{smallmatrix}, 1 \right), \\ F_{P+1,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_{N+1}, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi \end{smallmatrix}, 0 \right), \\ F_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi \end{smallmatrix}, 0 \right) \end{array} \right| \text{ and } \left| \begin{array}{l} F_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi \end{smallmatrix}, 1 \right), \\ F_{P+1,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_{N+1}, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi \end{smallmatrix}, 1 \right), \\ F_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi \end{smallmatrix}, 0 \right). \end{array} \right| \quad (2.154)$$

The multipoint continued fractions (2.154₁) and (2.154₂) are the multipoint Padé approximants to $f_1(z)$. Due to Theorem 2.10 for any permutations of $(\alpha_1, \alpha_2, \dots, \alpha_N)$ we have

$$F_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_1, x_2, \dots, x_N, \xi \end{smallmatrix}, j \right) = F_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi \end{smallmatrix}, j \right), \quad j = 0, 1, \quad (2.155)$$

$$F_{P+1,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_{N+1}, 1 \\ x_1, x_2, \dots, x_N, \xi \end{smallmatrix}, j \right) = F_{P+1,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_{N+1}, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi \end{smallmatrix}, j \right), \quad j = 0, 1.$$

On account of (2.154) and (2.155) the boundaries $\phi_{P,1} \left(z, \begin{smallmatrix} p_1, p_2, \dots, p_N, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \xi \end{smallmatrix}, u \right)$ do not depend on the order of $(\alpha_1, \alpha_2, \dots, \alpha_N)$, see (2.153). ■

By way of illustration of the Theorem 2.21 let us consider the rational Stieltjes function

$$f_1(z) = 0.1139240506 + \frac{1.833835939}{1 + 0.5296680395z} + \frac{0.3800408399}{1 + 0.06876441793z}. \quad (2.156)$$

From the input data

$$f_1(-1) \leq \infty, \quad f_1(4) = 1.000, \quad f_1(9) = 0.6666, \quad f_1(19) = 0.4444 \quad (2.157)$$

we compute the sequences of the bounding functions

$$F_{2,1} \left(z, \begin{matrix} 1,+1 \\ 4,-1 \end{matrix}, u \right), \quad F_{3,1} \left(z, \begin{matrix} 1,1,+1 \\ 4,9,-1 \end{matrix}, u \right), \quad F_{4,1} \left(z, \begin{matrix} 1,1,1,+1 \\ 4,9,19,-1 \end{matrix}, u \right); \quad (2.158)$$

$$F_{2,1} \left(z, \begin{matrix} 1,+1 \\ 19,-1 \end{matrix}, u \right), \quad F_{3,1} \left(z, \begin{matrix} 1,1,+1 \\ 19,4,-1 \end{matrix}, u \right), \quad F_{4,1} \left(z, \begin{matrix} 1,1,1,+1 \\ 19,4,9,-1 \end{matrix}, u \right). \quad (2.159)$$

For example the functions $F_{4,1} \left(z, \begin{matrix} 1,1,1,+1 \\ 4,9,19,-1 \end{matrix}, u \right)$ and $F_{4,1} \left(z, \begin{matrix} 1,1,1,+1 \\ 19,4,9,-1 \end{matrix}, u \right)$ are equal to

$$F_{4,1} \left(z, \begin{matrix} 1,1,1,+1 \\ 4,9,19,-1 \end{matrix}, u \right) = \frac{1.000}{1+(z-4)} \times \frac{0.100}{1+(z-9)} \times \frac{0.020}{1+(z-19)} \times \frac{0.030F_1(z+1,u)}{1}, \quad (2.160)$$

$$F_{4,1} \left(z, \begin{matrix} 1,1,1,+1 \\ 19,4,9,-1 \end{matrix}, u \right) = \frac{0.444}{1+(z-19)} \times \frac{0.0370}{1+(z-4)} \times \frac{0.022}{1+(z-9)} \times \frac{0.057F_1(z+1,u)}{1}.$$

The S -estimates given by (2.158) and (2.159) are depicted in Fig. 2.7. Note that the boundaries $F_{4,1} \left(z, \begin{matrix} 1,1,1,+1 \\ 4,9,19,-1 \end{matrix}, u \right)$ and $F_{4,1} \left(z, \begin{matrix} 1,1,1,+1 \\ 19,4,9,-1 \end{matrix}, u \right)$ coincide (cf. Eqs (2.160_{1,2})).

$$\left\{ F_{4,1} \left(z, \begin{matrix} 1,1,1,+1 \\ 4,9,19,-1 \end{matrix}, u \right), \quad u \in [-1, 1] \right\} = \left\{ F_{4,1} \left(z, \begin{matrix} 1,1,1,+1 \\ 19,4,9,-1 \end{matrix}, u \right), \quad u \in [-1, 1] \right\}. \quad (2.161)$$

2.6 Fundamental inequalities for multipoint Padé approximants

On account of (2.50) for $z = x \in [\xi, \infty) \in \mathbb{R}$ the inclusion region $\Phi_{P,1}(z)$ reduce to the sections lying on the real axis

$$\Phi_{P,1}(x) = \{w \in \mathbb{R} : w = F_{P,1}(x, u); \quad -1 \leq u \leq 0\}, \quad f_1(x) \in \Phi_{P,1}(x), \quad (2.162)$$

where (cf. (2.47))

$$F_{P,1}(x, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (x - x_k)} \times \frac{w_p(1 + u)}{1}. \quad (2.163)$$

Let us rewrite the formula (2.163) as follows

$$F_{P,1}(x, u) = \frac{g_1}{1 + (x - x_1)F_{P-1,2}(x, u)}, \quad F_{P-1,2}(x, u) = \frac{g_2}{1 + (x - x_1)F_{P-2,3}(x, u)},$$

$$, \dots, \dots, \quad F_{2,P-1}(x, u) = \frac{g_p}{1 + (x - x_N)F_{1,P}(x, u)}, \quad F_{1,P}(x, u) = w_p F_1(x - x_N)$$

$$F_1(x - x_N) = (1 + u), \quad -1 \leq u \leq 0, \quad \xi < x < \infty. \quad (2.164)$$

From (2.164) one obtains

$$\begin{aligned} \frac{\partial F_{P,1}(x, u)}{\partial u} &= -\frac{g_1(x - x_1)}{(1 + (x - x_1)F_{P-1,2}(x, u))^2} \frac{\partial F_{P-1,2}(x, u)}{\partial u} = \\ &\left(\frac{g_1(x - x_1)}{(1 + (x - x_1)F_{P-1,2}(x, u))^2} \right) \left(\frac{g_2(x - x_1)}{(1 + (x - x_1)F_{P-2,3}(x, u))^2} \right) \frac{\partial F_{P-2,3}(x, u)}{\partial u} \quad (2.165) \\ &=, \dots, = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \left(-\frac{g_j(x - x_k)}{(1 + (x - x_k)F_{P-j,1+j}(x, u))^2} \right) \frac{\partial F_{1,P}(x, u)}{\partial u}. \end{aligned}$$

The sign of $\partial F_{P,1}(x, u)/\partial u$ is given by

$$\text{sign} \left(\frac{\partial F_{P,1}(x, u)}{\partial u} \right) = \text{sign} \left(\prod_{k=1}^N \left(\prod_{P_{k-1}+1}^{P_k} (x_k - x) \right) \right), \quad \xi \leq x < \infty. \quad (2.166)$$

Simple rearrangements of (2.166) yield

$$\text{sign} \left(\frac{\partial F_{P,1}(x, u)}{\partial u} \right) = \text{sign} ((x_1 - x)^{p_1} (x_2 - x)^{p_2} \dots (x_N - x)^{p_N}) \quad (2.167)$$

or equivalently

$$\text{sign} \left(\frac{\partial F_{P,1}(x, u)}{\partial u} \right) = \begin{cases} (-1)^0 & \text{if } \xi < x < x_1, \\ (-1)^{P_1} & \text{if } x_1 < x < x_2, \\ \dots & \dots \\ (-1)^{P_N} & \text{if } x_N < x < \infty. \end{cases} \quad (2.168)$$

For a fixed x the function $F_{P,1}(x, u)$ is monotonic with respect to u (cf. (2.168)). Hence we have

$$\begin{aligned} (-1)^0 F_{P,1}(x, -1) &\leq (-1)^{P_0} f_1(x) & \text{if } \xi < x \leq x_1, \\ (-1)^{P_1} F_{P,1}(x, -1) &\leq (-1)^{P_1} f_1(x) & \text{if } x_1 \leq x \leq x_2, \\ \dots &\dots & \dots \\ (-1)^{P_N} F_{P,1}(x, -1) &\leq (-1)^{P_N} f_1(x) & \text{if } x_N \leq x < \infty \end{aligned} \quad (2.169)$$

and

$$\begin{aligned} (-1)^0 F_{P,1}(x, 0) &\leq (-1)^{P_0+1} f_1(x) & \text{if } \xi < x \leq x_1, \\ (-1)^{P_1} F_{P,1}(x, 0) &\leq (-1)^{P_1+1} f_1(x) & \text{if } x_1 \leq x \leq x_2, \\ \dots &\dots & \dots \\ = (-1)^{P_N} F_{P,1}(x, 0) &\leq (-1)^{P_N+1} f_1(x) & \text{if } x_N \leq x < \infty, \end{aligned} \quad (2.170)$$

where $P_j, j = 1, 2, \dots, N$ and P are defined by (2.14). From the relations (2.169) and (2.170), it follows the fundamental S -inequalities for diagonal and overdiagonal multipoint Padé approximants $F_{P,1}(x, j), j = 0, 1$ (cf. Theorem (2.22))

Theorem 2.22 Consider the non-decreasing power series of Stieltjes (cf. Definition 2.4)

$$f_1(x) = \sum_{i=0}^{p_j} c_{ij}(x - x_j)^i + O((x - x_j)^{p_j}), \quad j = 1, \dots, N; \quad f_1(x) = \eta + O(x - \xi) \quad (2.171)$$

and accompanying them the $L_P(x)$ characteristic functions, cf. (2.6). For fixed ξ and η the diagonal and overdiagonal multipoint Padé approximants $F_{P,1}(x, J)$, $x \in \mathbb{R} \setminus [-\infty, \xi]$, $J = 0, -1$ to the power expansions (2.171) satisfy the following inequalities

$$\begin{aligned} (-1)^{L_{P-1}(x)} F_{P-1,1}(x, 0) &\leq (-1)^{L_{P-1}(x)} F_{P,1}(x, 0), \\ (-1)^{L_{P-1}(x)} F_{P-1,1}(x, -1) &\geq (-1)^{L_{P-1}(x)} F_{P,1}(x, -1), \end{aligned} \tag{2.172}$$

$$(-1)^{L_P(x)} F_{P,1}(x, 0) \leq (-1)^{L_P(x)} f_1(x) \leq (-1)^{L_P(x)} F_{P,1}(x, -1).$$

Proof. From (2.170) and Theorem 2.17 the inequalities (2.172) follows at once.

■

The relations (2.172) have a consequence that the multipoint Padé approximants $F_{P,1}(x, J)$, $J = -1, 0$ form the optimum upper and lower bounds on $f_1(x)$ obtainable using only the given number of coefficients (P is fixed, Theorem 2.12). The use of additional coefficients (higher P) improves the bounds $F_{P,1}(x, J)$, $J = -1, 0$ on $f_1(x)$.

Theorems 2.12 and 2.22 are fundamental, for they provide the best bounds on a Stieltjes function $f_1(z)$ from the truncated power series expanded at number of real points. For one-point Padé approximants the relations (2.172) reduce to the classical estimates of $f_1(x)$ derived by Baker in [9, Th.5.22, Th.5.42]. Moreover, the inequalities for multipoint Padé approximants derived in [28, 69, 70, 71] are the particular cases of the general relations (2.172).

Now we evaluate the estimates $F_{P,1}(x, 0)$ and $F_{P,1}(x, -1)$ of a Stieltjes function $f_1(x)$, $x \in \mathbb{R}$ for the following particular cases.

Stieltjes function expanded at zero

(a) The first term is available only Let the truncated power expansions $f_1(x)_x^p$ of a Stieltjes function $f_1(x)$

$$f_1(x) = f_1(x)_x^p, \quad \binom{p}{x} = \binom{1}{0} \tag{2.173}$$

be given. The parametric series associated with the initial input ones (2.173) are equal to (cf. (2.70))

$$f_1^{\xi, \eta}(x) = f_1^{\xi, \eta}(x)_x^p, \quad \binom{p}{x} = \binom{1, 1}{0, \xi} \tag{2.174}$$

or explicitly

$$f_1^{\xi, \eta}(x) = g_1 + O(x - 0), \quad f_1^{\xi, \eta}(x) = \eta + O(x - \xi), \quad \xi < 0, \quad g_1 \leq \eta, \quad \xi \geq x. \tag{2.175}$$

From (2.174) and (2.163), it follows

$$F_{2,1}^{\xi, \eta}(x, u) = \frac{g_1}{1 + x F_{1,2}^{\xi, \eta}(x, u)}, \quad F_{1,2}^{\xi, \eta}(x, u) = w_2^{\xi, \eta}(1 + u), \quad -1 \leq u \leq 0. \tag{2.176}$$

Relations (2.174), (2.175) and (2.176) yield

$$F_{2,1}^{\xi, \infty}(x, u) = \frac{g_1}{1 + x w_2^{\xi, \infty} F_1(x, u)}, \quad \frac{g_1}{1 + \xi w_2^{\xi, \infty}} = \infty, \quad w_2^{\xi, \infty} = -\frac{1}{\xi}. \tag{2.177}$$

Thus we have at once

$$F_{2,1}^{\xi, \infty}(x, u) = \lim_{\xi \rightarrow 0} \left(\frac{g_1}{1 - \frac{x}{\xi}(1 + u)} \right) = g_1 F_2(x, \tau), \quad -1 \leq u, \tau \leq 0, \tag{2.178}$$

where

$$F_2(x, \tau) = -g_1\tau, \quad -1 \leq \tau \leq 0. \quad (2.179)$$

The equation (2.179₁) leads to

$$F_{2,1}(x, -1) = g_1, \quad F_{2,1}(x, 0) = 0, \quad L_2(x) = 2H(x), \quad (2.180)$$

where $H(x)$ is a Heavisidea function, cf. (1.52). From (2.180) and (2.172), it follows immediately that

$$(-1)^{2H(x)}F_{2,1}(x, 0) \leq (-1)^{2H(x)}f_1(x) \leq (-1)^{2H(x)}F_{2,1}(x, -1). \quad (2.181)$$

Finally we obtain

$$0 \leq f_1(x) \leq g_1, \quad x > 0. \quad (2.182)$$

It is worth to notice that the relation (2.182) can be obtained directly from the formulae (2.97) and (2.98) via replacing of a complex variable z by the real one x .

Stieltjes function expanded at a number of real points

(b) The case $\xi < \mathbf{x}_N = \min(\mathbf{x}_j, j = 1, 2, \dots, N)$ For the assumptions **(b)** and the input data given by

$$f_1(z) \underset{\mathbf{x}}{P}, \underset{\mathbf{x}}{(P)} = \left(\begin{array}{c} p_1, p_2, \dots, p_N \\ x_1, x_2, \dots, x_N \end{array} \right) \quad (2.183)$$

the bounds $F_{P,1}^{x_N, \infty}(x, 0)$ and $F_{P,1}^{x_N, \infty}(x, 1)$ on $f_1(x)$ are equal to (cf. (2.108))

$$F_{P,1}^{x_N, \infty}(x, \tau) = \bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k - \delta_{kN}} \frac{g_j^{x_N}}{1 + (x - x_k)} \times \frac{(-g_{P-1}^{x_N} \tau)}{1}, \quad -1 \leq \tau \leq 0. \quad (2.184)$$

The fundamental S -inequalities (2.172) take the form

$$(-1)^{L_P(x)} F_{P,1}^{x_N, \infty}(x, 0) \leq (-1)^{L_P(x)} f_1(x) \leq (-1)^{L_P(x)} F_{P,1}^{x_N, \infty}(x, -1). \quad (2.185)$$

(c) The case $\xi < \mathbf{x}_1 = \min(\mathbf{x}_j, j = 1, 2, \dots, N)$ From the power series (2.183) and accompanying them the assumptions **(c)** we obtain (see (2.113))

$$F_{P,1}^{x_1, \infty}(x, u) = \bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \frac{g_j^{x_1}}{1 + (x - x_k)} \times \frac{w_P^{x_1}(1 + u)}{1}, \quad -1 \leq u \leq 0. \quad (2.186)$$

The bounding functions $F_{P,1}^{x_1, \infty}(x, 0)$ and $F_{P,1}^{x_1, \infty}(x, -1)$ satisfy the fundamental inequalities (2.172)

$$(-1)^{L_P(x)} F_{P,1}^{x_1, \infty}(x, 0) \leq (-1)^{L_P(x)} f_1(x) \leq (-1)^{L_P(x)} F_{P,1}^{x_1, \infty}(x, -1). \quad (2.187)$$

(d) The cases $\xi < \mathbf{x}_N = \min(\mathbf{x}_j, j = 1, 2, \dots, N-1)$ and $\xi < \mathbf{x}_1 = \min(\mathbf{x}_j, j = 2, 3, \dots, N)$ Let us turn our attention to the bounding functions $F_{P,1}^{x_N, \infty}(x, 0)$, $F_{P,1}^{x_N, \infty}(x, -1)$ (2.184) and $F_{P,1}^{x_1, \infty}(x, 0)$, $F_{P,1}^{x_1, \infty}(x, -1)$ (2.186). They are the best over the input data given by (2.183), so they should coincide. From the Theorem 2.21, it follows at once

$$F_{P,1}^{x_N, \infty}(x, -1) = F_{P,1}^{x_1, \infty}(x, -1) \quad \text{and} \quad F_{P,1}^{x_N, \infty}(x, 0) = F_{P,1}^{x_1, \infty}(x, 0). \quad (2.188)$$

As an example we consider the sequences $f_1(x)_{x_1}^1$ and $f_1(x)_{x_2}^1$ of truncated power expansions of $f_1(x)$

$$f_1(x)_{x_1}^1 = 1 + O(x - x_1) \text{ and } f_1(x)_{x_2}^1 = \frac{1}{7} + O(x - x_2), \quad x_1 = 0, \quad x_2 = 3 \quad (2.189)$$

and

$$f_1(x)_{x_1}^1 = \frac{1}{7} + O(x - x_1) \text{ and } f_1(x)_{x_2}^1 = 1 + O(x - x_2), \quad x_1 = 3, \quad x_2 = 0. \quad (2.190)$$

For (2.189) and (2.190) the bounding functions are equal to

$$F_{3,1}^{x_1,\infty}(x, u) = \frac{1}{1 + \frac{1}{\frac{2x}{1 + \frac{1}{3}(x-3)(1+u)}}} \quad \text{and} \quad F_{3,1}^{x_2,\infty}(x, \tau) = \frac{\frac{1}{7}}{1 - \frac{2}{7}(x-3)\tau}. \quad (2.191)$$

It can be easily checked that if $u, \tau = -1, 0$ we have

$$\begin{aligned} F_{3,1}^{x_1,\infty}(x, -1) &= \frac{1}{1 + 2x} = F_{3,1}^{x_2,\infty}(x, -1) = \frac{1}{1 + 2x}, \\ F_{3,1}^{x_1,\infty}(x, 0) &= \frac{1}{7} = F_{3,1}^{x_2,\infty}(x, 0) = \frac{1}{7}. \end{aligned} \quad (2.192)$$

In spite of the seemingly unsymmetrical structures of the bounding functions $F_{3,1}^{x_1,\infty}(x, J)$ and $F_{3,1}^{x_2,\infty}(x, J)$, $J = -1, 0$ the identities

$$F_{3,1}^{x_1,\infty}(x, -1) = F_{3,1}^{x_2,\infty}(x, -1) \text{ and } F_{3,1}^{x_1,\infty}(x, 0) = F_{3,1}^{x_2,\infty}(x, 0) \quad (2.193)$$

are satisfied.

As an example illustrating Theorem 2.22 we consider the truncated power expansions

$$\begin{aligned} f_1(x)_{10^1}^2 &= 0.1792 + 0.00958(x - 10) + O((x - 10)^2), \\ f_1(x)_{10^4}^2 &= 0.0008 + 0.7517(x - 10^4) + O((x - 10^4)^2) \end{aligned} \quad (2.194)$$

of a Stieltjes function

$$f_1(x) = \frac{1}{x} \ln(0.5(x + 2)). \quad (2.195)$$

The parametric power series added to the input data (2.194) takes the form

$$f_1(x)_\xi^1 = \eta + O(x - \xi). \quad (2.196)$$

According to (2.184) the multipoint Padé approximants

$$F_{4,1}(x, 0), F_{4,1}(x, -1) \text{ and } F_{5,1}(x, 0), F_{5,1}(x, -1) \quad (2.197)$$

are the best estimations of $f_1(x)$ (2.195) constructed from the coefficients

$$c_{01} = 0.1792, \quad c_{11} = .00958, \quad c_{02} = 0.0008 \quad (2.198)$$

and

$$c_{01} = 0.1792, \quad c_{11} = .00958, \quad c_{02} = 0.0008, \quad c_{12} = 0.7517, \quad (2.199)$$

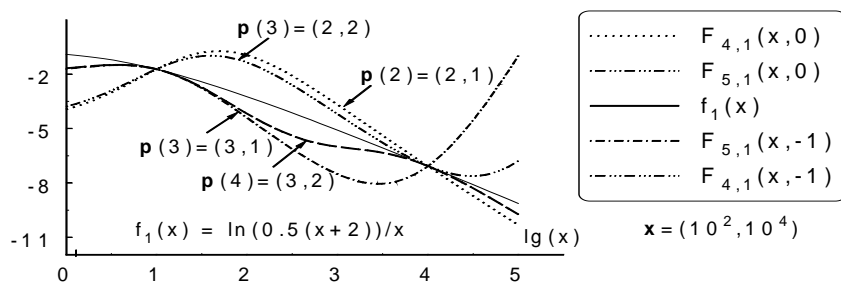


Fig. 2.8 Sequence of Padé approximants $F_{4,1}(x, 0)$, $F_{4,1}(x, -1)$ and $F_{5,1}(x, 0)$, $F_{5,1}(x, -1)$ forming the upper and lower bounds on the Stieltjes function $\ln(0.5(x+2))/x$, cf. Th. 2.22.

respectively. The multipoint Padé approximants (2.197) satisfy the fundamental inequalities (2.185)

$$\begin{aligned} (-1)^{L_4(x)} F_{4,1}(x, 0) &\leq (-1)^{L_4(x)} f_1(x) \leq (-1)^{L_4(x)} F_{4,1}(x, -1), \\ (-1)^{L_5(x)} F_{5,1}(x, 0) &\leq (-1)^{L_5(x)} f_1(x) \leq (-1)^{L_5(x)} F_{5,1}(x, -1), \end{aligned} \quad (2.200)$$

where

$$L_4(x) = 3H(x - 10) + H(x - 10^4) \text{ and } L_5(x) = 3H(x - 10) + 2H(x - 10^4). \quad (2.201)$$

Figure (2.8) presents the bounds $F_{4,1}(x, 0)$, $F_{4,1}(x, -1)$ and $F_{5,1}(x, 0)$, $F_{5,1}(x, -1)$ on $f_1(x)$.

2.7 Summary and final remarks about SMC FM

In this chapter we derived the S - Multipoint Continued Fraction Method of an estimation a Stieltjes function $f_1(z)$ from the incomplete power series $f_1(z)_x^p$ constructed at real points $x_1, x_2, x_3, \dots, x_N$, where $\max(x_1, x_2, x_3, \dots, x_N) < \infty$. We proved that the S -estimates of $f_1(z)$ obtained via SMC FM are the best with respect to the truncated power series $f_1(z)_x^p$. This important results is new.

The real parameters ξ, η (2.2), the recurrence S -algorithm (2.13)- (2.14), the fundamental S - inclusion relations (2.84)-(2.85) and the general S - inequalities (2.172) are the main mathematical tools of the SMC FM.

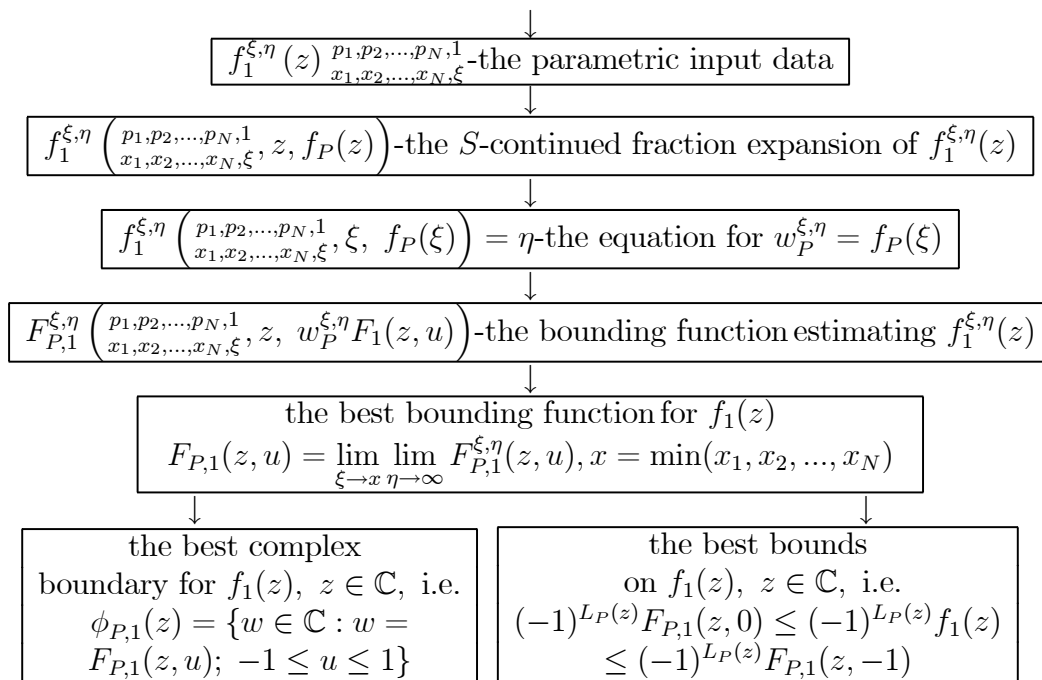
The algorithm (2.13)-(2.14) transforms the truncated power series (2.88) first to the bounding functions (2.90) next to the complex boundaries (2.49) and finally, if $f_1(z) \in \mathbb{C}$ to the best inclusion regions (2.50) or if $f_1(z) \in \mathbb{R}$ to the best upper and lower bounds on $f_1(z)$ (2.172).

From the fundamental S -inclusion relations (2.84)-(2.85) and the general S -inequalities (2.172), it follows the values of the parameters ξ and η (2.2) optimizing bounds on $f_1(z)$ in both complex (via 2.91), (2.84)-(2.85)) and real (via 2.91), (2.172) domains.

The problems of an approximation of a Stieltjes function $f_1(z)$ from the truncated power series $f_1(z)$ exploited before in [6, 9, 10, 24, 26, 27, 28, 53, 54, 55] dealt with limited numbers of coefficients of the power expansions of $f_1(z)$, see also [6, Chap.17].

The SMC FM established here is a first method of the theory of an approximation of Stieltjes functions, that incorporates into the estimates of $f_1(z)$ the power series consisting of arbitrary numbers of terms. The computational block diagram representing the SMC FM is as follows:

$$f_1(z) = f_1(z)_{x_1, x_2, \dots, x_N}^{p_1, p_2, \dots, p_N} \text{-the initial input data}$$



Among many unquestionable advantages the SMCFM has one essential disadvantage. It does not work with the truncated power series expanded at infinity. In the next chapter we overcome this disadvantage by establishing the T -Multipoint Continued Fraction Method (TMCFM) of estimation of a Stieltjes function.

Chapter 3

THE BEST ESTIMATES OF A STIELTJES FUNCTION EXPANDED AT REAL POINTS AND INFINITY

The aim of this chapter is to derive in a unified and coherent form the T -Multipoint Continued Fraction Method (TMC FM) of an estimation of a Stieltjes function $f_1(z)$ from the truncated power series expanded at real points x_1, x_2, \dots, x_N , infinity $x_{N+1} = \infty$ and $\xi < \min(x_1, x_2, \dots, x_N)$. The first letter T appearing in TMC FM follows from Thron, who first derived two-point continued fractions to analytical functions, cf. [31].

The TMC FM is the first method of the theory of an approximation of Stieltjes functions, that incorporates into the estimates of $f_1(z)$ the truncated power series $f_1(z)$ expanded at infinity, cf. [6, 9, 24, 27, 53, 54, 55, 66, 67, 68]. If the power expansion of $f_1(z)$ at $z = \infty$ is unknown the TMC FM reduces to the SMC FM established in Chapter 3.

In the sequel the TMC FM is adapted for estimating of the effective transport coefficients of two-phase media.

3.1 The T-multipoint continued fraction expansions of a Stieltjes function.

3.1.1 Power expansions of a Stieltjes function at infinity

The following Lemma is a starting point for an estimation of a Stieltjes function $f_1(z)$ from its power expansions available at a number of real points and infinity.

Lemma 3.1 *If $f_1(z)$ is a Stieltjes function*

$$f_1(z) = \int_{1/\varrho_\infty}^{1/\varrho_0} \frac{d\gamma_1(u)}{1+zu}, \quad d\gamma_1(u) \geq 0, \quad 0 < \varrho_0 < \varrho_\infty, \quad (3.1)$$

then $\varphi_1(s)$ defined by

$$\varphi_1(s) = \int_{\varrho_0}^{\varrho_\infty} \frac{d\gamma_\infty(u)}{1+su}, \quad d\gamma_\infty(u) \geq 0, \quad 0 < \varrho_0 < \varrho_\infty \quad (3.2)$$

is also a Stieltjes function, provided that

$$f_1(z) = s\varphi_1(s), \quad z = \frac{1}{s}, \quad (3.3)$$

where

$$d\gamma_\infty(u) = -ud\gamma_1\left(\frac{1}{u}\right). \quad (3.4)$$

Proof. By substituting $z = 1/s$ into (3.1) we arrive at (3.2)-(3.4) immediately. ■

Remark 3.2 *Since $f_1(z)$ and $\varphi_1(s)$ are Stieltjes functions any estimation procedures constructed for $f_1(z)$ are valid (after simple adaptation) for $\varphi_1(s)$ as well, cf. (3.1)-(3.4).*

In this section we limit our investigations to Stieltjes functions $f_1(z)$ represented by the power series with non-zero radii of convergence $1/\varrho_\infty > 0$, see (3.1)-(3.4). Consider the power expansions:

Of $f_1(z)$ at $z = x_N$,

$$f_1(z) = \sum_{i=0}^{\infty} c_{iN} (z - x_N)^i, \quad -\varrho_0 < z < 2(x_N + \varrho_0). \quad (3.5)$$

Of $\varphi_1(s)$ at $s = y_N$

$$\varphi_1(s) = \sum_{i=0}^{\infty} d_{iN} (s - y_N)^i, \quad -\frac{1}{\varrho_\infty} < s < 2(y_N + \frac{1}{\varrho_\infty}). \quad (3.6)$$

Of $s\varphi_1(s)$ at $s = y_N$

$$s\varphi_1(s) = \sum_{i=0}^{\infty} b_{iN} (s - y_N)^i, \quad -\frac{1}{\varrho_\infty} < s < 2(y_N + \frac{1}{\varrho_\infty}). \quad (3.7)$$

Here x_N and y_N are real numbers. The intervals of a convergence of the power series $f_1(z)$ (3.5₁), $\varphi_1(s)$ (3.6₁) and $s\varphi_1(s)$ (3.7₁) follow directly from the inequalities (1.69)-(1.70). The substitution into (3.5)- (3.7)

$$s = \frac{1}{z}, \quad y_N = \frac{1}{x_N}, \quad (3.8)$$

allows us to write the equalities

$$f_1(z) = \sum_{i=0}^{\infty} c_{iN} (z - x_N)^i = \sum_{i=0}^{\infty} b_{iN} \left(\frac{1}{z} - \frac{1}{x_N}\right)^i = \frac{1}{z} \sum_{i=0}^{\infty} d_{iN} \left(\frac{1}{z} - \frac{1}{x_N}\right)^i \quad (3.9)$$

valid for z satisfying

$$\frac{1}{\frac{2}{x_N} + \frac{2}{\varrho_\infty}} < z < 2(x_N + \varrho_0). \quad (3.10)$$

The coefficients b_{iN} , d_{iN} and c_{iN} appearing in (3.9) are interrelated by the recurrence formula derived in Section ?? of the Appendix

$$\begin{aligned} b_0 &= c_0, \quad b_n = \frac{(-1)^n}{n!} \sum_{i=1}^n \frac{(n+1-i)! c_{n+1-i} r_{n,i}}{y^{2n+1-i}}, \quad n = 1, 2, \dots, \\ c_0 &= b_0, \quad c_n = \frac{(-1)^n}{n!} \sum_{i=1}^n \frac{(n+1-i)! b_{n+1-i} r_{n,i}}{x^{2n+1-i}}, \quad n = 1, 2, \dots, \end{aligned} \quad (3.11)$$

where

$$\begin{aligned} b_n &= yd_n + d_{n-1}, \quad n = 1, 2, \dots, \\ d_{-1} &= 0, \quad d_n = \frac{b_n - d_{n-1}}{y}, \quad n = 1, 2, \dots, \end{aligned} \quad (3.12)$$

and

$$\left. \begin{aligned} r_{j-1,0} &= 0, \quad r_{j-1,1} = 1, \quad r_{j-1,j+1} = 0, \\ r_{j,k} &= 2(j-k)r_{j-1,k-1} + r_{j-1,k}, \quad k = 1, 2, \dots, j+1. \end{aligned} \right\}, \quad j = 1, 2, \dots, n. \quad (3.13)$$

For $i = 1, 2$ the formulae (3.11)-(3.13) reduce to the following relations

$$\begin{aligned} r_{0,0} &= 0, \quad r_{0,1} = 1, \quad r_{0,2} = 0, \quad r_{1,1} = r_{0,1} = 1, \\ b_0 &= c_0, \quad b_1 = -\frac{c_1}{y^2}; \quad d_0 = \frac{b_0}{y}, \quad d_1 = \frac{b_1}{y} - \frac{b_0}{y^2}; \\ c_0 &= \frac{d_0}{x}, \quad c_1 = -\frac{d_0x + d_1}{x^3}; \quad y = \frac{1}{x}. \end{aligned} \tag{3.14}$$

Note that in (3.11)-(3.14) the index N is omitted, cf. (3.9).

Now we focus our attention on the Stieltjes series represented by (3.9₁) and (3.9₃) only. The equality (3.9) leads to the following conclusion

Conclusion 3.3 *If $z > \frac{\varrho_\infty}{2}$ and $x_N \rightarrow \infty$ then*

$$f_1(z) = \frac{1}{z} \sum_{i=0}^{\infty} d_i(\infty) \left(\frac{1}{z}\right)^i = \frac{1}{z} \sum_{i=0}^{\infty} d_i(x_N) \left(\frac{1}{z} - \frac{1}{x_N}\right)^i = \sum_{i=0}^{\infty} c_i(x_N) (z - x_N)^i, \tag{3.15}$$

where $d_i(x_N)$ and $c_i(x_N)$ are interrelated by (3.11)-(3.13).

By replacing in (3.15) $d_i(x_N)$ by $d_i(\infty)$ and $c_i(x_N)$ by $c_i^\infty(x_N)$ we arrive at:

Conclusion 3.4 *If $z > \frac{\varrho_\infty}{2}$ and $x_N \rightarrow \infty$ then*

$$f_1(z) = \frac{1}{z} \sum_{i=0}^{\infty} d_i(\infty) \left(\frac{1}{z}\right)^i = \frac{1}{z} \sum_{i=0}^{\infty} d_i(\infty) \left(\frac{1}{z} - \frac{1}{x_N}\right)^i = \sum_{i=0}^{\infty} c_i^\infty(x_N) (z - x_N)^i, \tag{3.16}$$

where $d_i(\infty)$ and $c_i^\infty(x_N)$ are given by (3.11)-(3.13).

From the infinite power series (3.16), it follows immediately:

Conclusion 3.5 *If $x_N \rightarrow \infty$ and $|z - x_N| \rightarrow 0$ then*

$$\begin{aligned} f_1(z) &= \frac{1}{z} \sum_{i=0}^{p_\infty-1} d_i(\infty) \left(\frac{1}{z}\right)^i + O\left(\left(\frac{1}{z}\right)^{p_\infty}\right) \\ &= \sum_{i=0}^{p_\infty-1} c_i^\infty(x_N) (z - x_N)^i + O((z - x_N)^{p_\infty}), \end{aligned} \tag{3.17}$$

provided $d_i(\infty)$ and $c_i^\infty(x_N)$ satisfy (3.11)-(3.13).

The equality (3.17) motivates us to introduce:

Definition 3.6 *The truncated power series (3.17₁) and (3.17₂) with the coefficients $d_i(\infty)$ and $c_i^\infty(x_N)$ interrelated by (3.11)-(3.13) we call the interchangeable ones.*

Now we are ready to present the main result of this section:

Theorem 3.7 Consider two sets of truncated power series (cf. (2.4))

$$f_1(z) = f_1(z)_{x_1, x_2, \dots, x_{N-1}, \infty, \xi}^{p_1, p_2, \dots, p_{N-1}, p_\infty, 1} \quad \text{and} \quad f_1^{x_N}(z) = f_1^{x_N}(z)_{x_1, x_2, \dots, x_{N-1}, x_N, \xi}^{p_1, p_2, \dots, p_{N-1}, p_\infty, 1}, \quad (3.18)$$

where the following ones coincide

$$f_1(z)_{x_1, x_2, \dots, x_{N-1}, \xi}^{p_1, p_2, \dots, p_{N-1}, 1} = f_1^{x_N}(z)_{x_1, x_2, \dots, x_{N-1}, \xi}^{p_1, p_2, \dots, p_{N-1}, 1}, \quad (3.19)$$

while the remaining $f_1(z)_\infty^{p_\infty}$ (see (3.18₁)) and $f_1^{x_N}(z)_{x_N}^{p_\infty}$ (see (3.18)₂) take the forms

$$f_1(z)_\infty^{p_\infty} = \frac{1}{z} \sum_{i=0}^{p_\infty-1} d_i(\infty) \left(\frac{1}{z}\right)^i + O\left(\left(\frac{1}{z}\right)^{p_\infty}\right) \quad (3.20)$$

and

$$f_1^{x_N}(z)_{x_N}^{p_\infty} = \sum_{i=0}^{p_\infty-1} c_i^\infty(x_N) (z - x_N)^i + O((z - x_N)^{p_\infty}). \quad (3.21)$$

If the expansions (3.20) and (3.21) are interchangeable (see Definition 3.6) then the bounding function $F_{P_\infty, 1}(z, u)$ computed from (3.18₁) and the bounding one $F_{P_\infty, 1}^{x_N}(z, u)$ generated by (3.18₂) satisfy the relations (cf. 2.48)

$$F_{P_\infty, 1}(z, u) = F_{P_\infty, 1}^{x_N}(z, u), \quad x_N \rightarrow \infty, \quad P^\infty = \sum_{i=1}^{N-1} p_i + p_\infty + 1. \quad (3.22)$$

Proof. Due to Theorem (3.11) the bounding functions $F_{P_\infty, 1}^{x_N}(z, u)$ and $F_{P_\infty, 1}(z, u)$ are defined by

$$F_{P_\infty, 1}^{x_N}(z, u) - \sum_{i=0}^{p_\infty-1} c_i^\infty(x_N) (z - x_N)^i = O((z - x_N)^{p_\infty}), \quad -1 \leq u \leq 1 \quad (3.23)$$

and

$$F_{P_\infty, 1}(z, u) - \frac{1}{z} \sum_{i=0}^{\infty} d_i(\infty) \left(\frac{1}{z}\right)^i = \frac{1}{z} O\left(\left(\frac{1}{z}\right)^{p_\infty}\right), \quad -1 \leq u \leq 1. \quad (3.24)$$

Since the power series (3.20) and (3.21) are interchangeable the following equality is true (cf. (3.17))

$$\frac{1}{z} \left(\sum_{i=0}^{\infty} d_i(\infty) \left(\frac{1}{z}\right)^i + O\left(\left(\frac{1}{z}\right)^{p_\infty}\right) \right) = \sum_{i=0}^{p_\infty-1} c_i^\infty(x_N) (z - x_N)^i + O((z - x_N)^{p_\infty}) \quad (3.25)$$

$$\sum_{i=0}^{p_\infty-1} c_i^\infty(x_N) (z - x_N)^i + O((z - x_N)^{p_\infty}) \quad \text{for } x_N \rightarrow \infty \text{ and } |z - x_N| \rightarrow 0.$$

Thus from (3.23), (3.24) and 3.25), it follows the identity (3.22). ■

By way of illustration of Theorem 3.7 we consider the truncated power series

$$f_1(z) = \frac{1}{z} \left(d_0(\infty) + d_1(\infty) \left(\frac{1}{z}\right) + O\left(\left(\frac{1}{z}\right)^2\right) \right) \quad (3.26)$$

and

$$f_1^{x_N}(z) = c_0^\infty(x_N) + c_1^\infty(x_N) (z - x_N) + O((z - x_N)^2), \quad (3.27)$$

where

$$c_0^\infty(x_N) = \frac{d_0(\infty)}{x_N}, \quad c_1^\infty(x_N) = -\frac{d_0(\infty)x_N + d_1(\infty)}{x_N^3}. \quad (3.28)$$

One can easily check that series (3.26) and (3.27)-(3.28) are interchangeable, see (3.14₃).

$$f_1(z) = \bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{f_P(z)}{1}, \quad (3.35)$$

$$f_P(z) = W_P(e_P) + O(z - \xi), \quad W_P = w_P - e_P, \quad W_P = f_P(\xi).$$

The alternative notations for (3.35), namely

$$\begin{aligned} & \bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{f_P(z)}{1} \\ &= \mathbf{T}_{P-1} f_P(z) = \bigvee_{k=1}^N \mathbf{T}_{P_{k-1}+1}^{P_k} f_P(z), \end{aligned} \quad (3.36)$$

and

$$\bigvee_{k=1}^N \bigvee_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{f_P(z)}{1} = \quad (3.37)$$

$$f_1(z, \mathbf{p}, f_P(z)) = f_1\left(z, \begin{matrix} p_1, p_2, \dots, p_N, p_\infty, 1 \\ x_1, x_2, \dots, x_N, \infty, \xi \end{matrix}, f_P(z)\right)$$

will also be used. As an example let us evaluate the T -continued fraction expansion of

$$f_1(z) = \frac{1}{z} \left(1 + \frac{2.5}{z} \ln \left(\frac{1 + 0.1z}{1 + 0.5z} \right) \right) \quad (3.38)$$

from the truncated power series

$$f_1(z) \mathbf{p}_x, \left(\mathbf{p}_x \right) = \left(\begin{matrix} 1, 1, 2, +1 \\ 2, 5, \infty, -1 \end{matrix} \right). \quad (3.39)$$

Formulae (3.39) and (3.38) yield

$$\begin{aligned} f_1(z)_2^1 &= 0.1807 + O(z - 2); \quad f_1(z)_5^1 = 0.1153 + O(z - 5); \\ z f_1(z)_\infty^2 &= 1 - 4.0236 \left(\frac{1}{z} \right) + O \left(\frac{1}{z} \right)^2; \quad f_1(z)_{-1}^{+1} = 0.4695 + O(z + 1). \end{aligned} \quad (3.40)$$

The recurrence relations (3.32) and the input data (3.40) lead to the following continued fraction expansion of $f_1(z)$ (cf. (3.35))

$$\begin{aligned} f_1(z) &= f_1\left(z, \begin{matrix} 1, 1, 2, +1 \\ 2, 5, \infty, -1 \end{matrix}, f_3(z)\right) = \\ &= \frac{g_1}{1 + e_2(z - 2) + (z - 2)} \times \frac{g_2}{1 + e_3(z - 5) + (z - 5)} \times \frac{f_3(z)}{1} = \\ &= \frac{g_1}{1 + e_2(z - 2) + \frac{(z - 2)g_2}{1 + e_3(z - 5) + (z - 5)f_3(z)}}, \quad f_3(z) = W_3 + O(z + 1), \end{aligned} \quad (3.41)$$

where

g_1	e_2	g_2	e_3	W_3	(3.42)
0.180733985	0.180733985	0.00857127	0.09666667	0.0111480	

3.1.3 Main properties of T -multipoint continued fraction expansions of a Stieltjes function

Now we prove theorems stating the most important properties of T -continued fraction expansion of $f_1(z)$ to $f_P(z)$, cf. Theorems 2.6, 2.7, 2.8, 1.16 and 2.10.

Theorem 3.9 *If $f_1(z)$ is a Stieltjes function*

$$f_1(z) = \int_0^{\infty} \frac{d\gamma_1(u)}{1+zu}, \quad \Delta\gamma_1(0) = 0, \quad (3.43)$$

then the tail $f_P(z)$ of a continued fraction expansion of $f_1(z)$

$$f_1(z) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1+(z-x_k)e_{j+1}+(z-x_k)} \times \frac{f_P(z)}{1}, \quad f_P(\xi) = W_P(e_P) \quad (3.44)$$

is also a Stieltjes function

$$f_P(z) = \int_0^{\infty} \frac{d\gamma_P(u)}{1+zu}, \quad \Delta\gamma_P(0) = 0. \quad (3.45)$$

Here $\Delta\gamma_j(0) = \gamma_j(0_+) - \gamma_j(0_-)$, $j = 1, 2, \dots, p$ denote the jumps of $\gamma_j(u)$ at $u = 0$.

Proof. By applying the linear fractional transformation (1.107) to the function $f_1(z)$ P_N times we arrive at the relation (3.44). The Stieltjes integral (3.45₁) and the relation (3.45₂) result directly from Theorem (1.9). ■

The next Theorem is relevant to Theorem 3.9. It states:

Theorem 3.10 *If $f_P(z)$ is a Stieltjes function*

$$f_P(z) = \int_0^{\infty} \frac{d\gamma_P(u)}{1+zu}, \quad \Delta\gamma_P(0) = 0 \quad (3.46)$$

then $f_1(z)$ appearing in

$$f_1(z) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1+(z-x_k)e_{j+1}+(z-x_k)} \times \frac{f_P(z)}{1}, \quad f_P(\xi) = W_P(e_P) \quad (3.47)$$

is also a Stieltjes function

$$f_1(z) = \int_0^{\infty} \frac{d\gamma_1(u)}{1+zu}, \quad \Delta\gamma_1(0) = 0. \quad (3.48)$$

Here $\Delta\gamma_j(0) = \gamma_j(0_+) - \gamma_j(0_-)$, $j = 1, 2, \dots, p$ denote the jumps of $\gamma_j(u)$ at $u = 0$.

Proof. Theorem 3.10 is a direct consequence of Theorem 1.15 ■

Theorem 3.11 *Let the continued fraction expansion of a Stieltjes functions $f_1(z)$ to $f_P(z)$ be given*

$$f_1(z) = f_1 \left(z, \begin{matrix} p_1, p_2, \dots, p_N, p_{\infty}, 1 \\ x_1, x_2, \dots, x_N, \infty, \xi \end{matrix}, f_P(z) \right), \quad f_P(\xi) = W_P. \quad (3.49)$$

The low order derivatives of $f_1(z)$ (3.49)

$$\left. \frac{d^0 f_1(z)}{dz^0} \right|_{\xi}, \quad \left. \frac{d^0 f_1(z)}{dz^0} \right|_{x_k}, \quad \left. \frac{d^1 f_1(z)}{dz^1} \right|_{x_k}, \quad \dots, \quad \left. \frac{d^{p_k-1} f_1(z)}{dz^{p_k-1}} \right|_{x_k}, \quad k = 1, 2, \dots, N \quad (3.50)$$

do not depend on $f_P(z)$ satisfying (3.49₂).

Proof. The proof of the Theorem 3.11 is analogous to the proof of Theorem 2.8. ■

Theorem 3.12 *There is an one to one correspondence between Stieltjes functions*

$$f_1 \in \Gamma_{x_1, x_2, \dots, x_N, \infty, \xi}^{p_1, p_2, \dots, p_N, p_\infty, 1} \quad \text{and} \quad f_P \in \Gamma_\xi^1 \quad (3.51)$$

satisfying T -linear fractional transformation (3.44), where

$$\Gamma_{x_1, x_2, \dots, x_N, \infty, \xi}^{p_1, p_2, \dots, p_N, p_\infty, 1} = \left\{ f_1 ; f_1(z) = \int_0^\infty \frac{d\gamma_1(u)}{1+zu}, \quad f_1(z)_{x_1, x_2, \dots, x_N, \infty, \xi}^{p_1, p_2, \dots, p_N, p_\infty, 1}, \quad d\gamma_1(u) \geq 0 \right\} \quad (3.52)$$

and

$$\Gamma_\xi^1 = \left\{ f_P ; f_P(z) = \int_0^\infty \frac{d\gamma_P(u)}{1+zu}, \quad f(z)_{\xi}^1 = w_P + O(z - \xi), \quad d\gamma_P(u) \geq 0 \right\}. \quad (3.53)$$

Proof. Theorem 3.12 is a direct consequence of Theorems 1.16 and 3.11. ■

Theorem 3.13 *Let the continued fraction expansions of $f_1(z)$, i.e.*

$$f_1 \left(z, \begin{matrix} p_1, p_2, \dots, p_N, p_\infty, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi \end{matrix}, f_P^\alpha(z) \right) \quad \text{and} \quad f_1 \left(z, \begin{matrix} p_1, p_2, \dots, p_N, p_\infty, 1 \\ x_{\beta_1}, x_{\beta_2}, \dots, x_{\beta_N}, \infty, \xi \end{matrix}, f_P^\beta(z) \right), \quad (3.54)$$

where

$$f_P^\alpha(\xi) = W_P^\alpha \quad \text{and} \quad f_P^\beta(\xi) = W_P^\beta, \quad (3.55)$$

be given. For any permutations of $(\alpha_1, \alpha_2, \dots, \alpha_N)$ and $(\beta_1, \beta_2, \dots, \beta_N)$ of natural numbers $(1, 2, \dots, N)$ the following identities are true

$$f_1 \left(z, \begin{matrix} p_1, p_2, \dots, p_N, p_\infty, 1 \\ x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi \end{matrix}, W_P^\alpha \right) = f_1 \left(z, \begin{matrix} p_1, p_2, \dots, p_N, p_\infty, 1 \\ x_{\beta_1}, x_{\beta_2}, \dots, x_{\beta_N}, \infty, \xi \end{matrix}, W_P^\beta \right). \quad (3.56)$$

Proof. The fraction expansions $f_1 \left(z, \begin{matrix} p \\ x_\alpha \end{matrix}, f_P^\alpha(z) \right)$ and $f_1 \left(z, \begin{matrix} p \\ x_\beta \end{matrix}, f_P^\beta(z) \right)$ are evaluated for the Stieltjes function $f_1(z)$, see (3.54). Hence the rational functions $f_1 \left(z, \begin{matrix} p \\ x_\alpha \end{matrix}, W_P^\alpha \right)$ and $f_1 \left(z, \begin{matrix} p \\ x_\beta \end{matrix}, W_P^\beta \right)$ are T -continued fractions to each other, cf. (3.54)-(3.55). On account of that they coincide, cf. (3.56). ■

3.2 Fundamental relations for T -inclusion regions

Since $f_j(z)$, $j = 1, \dots, P_N$ and $f_P(z)$ appearing in (3.32) are Stieltjes functions the coefficients of T -continued fractions (3.35) satisfy the inequalities

$$g_i > 0, \quad e_{i+1} \geq 0, \quad i = 1, \dots, P_N, \quad w_P > 0. \quad (3.57)$$

The tail $f_P(z)$ is represented by (cf. (3.45))

$$f_P(z) = f_P(\xi) + O(z - \xi) = W_P + O(z - \xi). \quad (3.58)$$

The first order bounding function $F_{1,P}(z, u, e_P)$ is equal to (cf. (1.154))

$$F_{1,P}(z, u, e_P) = W_P(e_P)F_1(z - \xi, u), \quad (3.59)$$

while the $(P + p_\infty)$ -th order one (cf. (3.35)) takes the form

$$F_{P+p_\infty,1}(z, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k) \times \frac{F_{1,P}(z, u, e_P)}{1}}. \quad (3.60)$$

From (3.60), it follows that

$$\begin{aligned} \Phi_{P+p_\infty,1}(z) = \\ \left\{ w \in \mathbb{C} : w = \prod_{k=1}^N \mathbf{T}_{P_{k-1}+1}^{P_k} \tau F_{1,P}(z, u, e_P); 0 \leq \tau \leq 1, -1 \leq u \leq 1 \right\} \end{aligned} \quad (3.61)$$

and

$$\begin{aligned} \phi_{P+p_\infty,1}(z) = \\ \left\{ w \in \mathbb{C} : w = \prod_{k=1}^N \mathbf{T}_{P_{k-1}+1}^{P_k} F_{1,P}(z, u, e_P); -1 \leq u \leq 1 \right\}, \end{aligned} \quad (3.62)$$

where

$$f_1(z) \in \Phi_{P+p_\infty,1}(z). \quad (3.63)$$

Here $\Phi_{P+p_\infty,1}(z)$ is the $(P + p_\infty)$ -th order inclusion region, while $\phi_{P+p_\infty,1}(z)$ the $(P + p_\infty)$ -th order complex boundary.

Theorem 3.14 *The estimations of $f_1(z)$, i.e. $F_{P+p_\infty,1}(z, u)$ (3.60), $\Phi_{P+p_\infty,1}$ (3.61) and $\phi_{P+p_\infty,1}(z)$ (3.62) evaluated from the incomplete power expansions $f_1(z)_{x_1, x_2, \dots, x_N, \infty, \xi}^{p_1, p_2, \dots, p_N, p_\infty, 1}$ are the best.*

Proof. It follows directly from Corollary 1.22 and Theorem 3.12 ■

Now we establish the inclusion relations for T -inclusion regions estimating a complex Stieltjes function $f_1(z)$.

Theorem 3.15 *For $z \in \mathbb{C} \setminus (-\infty, \xi_2]$ the T -inclusion regions $\Phi_{P_I^\infty,1}^{\xi_1, \eta_1}(z)$ and $\Phi_{P_{II}^\infty,1}^{\xi_2, \eta_2}(z)$ constructed from the truncated non-decreasing power series of Stieltjes (see Definition 2.4)*

$$\begin{aligned} f_1^{\xi_1, \eta_1}(z)_x^{p(P_I^\infty)}, \quad (p(P_I^\infty))_x = (p_1(P_I^\infty), p_2(P_I^\infty), \dots, p_N(P_I^\infty), p_\infty(P_I^\infty), 1), \\ x_1, x_2, \dots, x_N, \infty, \xi_1 \\ f_1^{\xi_2, \eta_2}(z)_x^{p(P_{II}^\infty)}, \quad (p(P_{II}^\infty))_x = (p_1(P_{II}^\infty), p_2(P_{II}^\infty), \dots, p_N(P_{II}^\infty), p_\infty(P_{II}^\infty), 1), \\ x_1, x_2, \dots, x_N, \infty, \xi_1 \end{aligned} \quad (3.64)$$

$$P_I^\infty = \sum_{i=1}^N p_i(1) + 1 + p_\infty(1), \quad P_{II}^\infty = \sum_{i=1}^N p_i(2) + 1 + p_\infty(2)$$

satisfy the relations

$$f_1^{\xi_1, \eta_1}(z) \in \Phi_{P_I^\infty,1}^{\xi_1, \eta_1}(z) \subset \Phi_{P_{II}^\infty,1}^{\xi_2, \eta_2}(z), \quad (3.65)$$

provided that

$$\eta_1 \leq \eta_2, \quad \xi_1 \leq \xi_2, \quad P_{II}^\infty \leq P_I^\infty. \quad (3.66)$$

Proof. By replacing the S -inclusion regions $\Phi_{P_I,1}^{\xi_1, \eta_1}(z)$ and $\Phi_{P_{II},1}^{\xi_2, \eta_2}(z)$ appearing in (2.84) by the corresponding T -inclusions ones $\Phi_{P_I^\infty,1}^{\xi_1, \eta_1}(z)$ and $\Phi_{P_{II}^\infty,1}^{\xi_2, \eta_2}(z)$ we obtain the relations (3.65) and (3.65) at once. It is justified by Theorem 3.7. ■

For fixed ξ and η the T -inclusion region $\Phi_{P^\infty,1}^{\xi, \eta}(z)$ forms the optimum estimate of $f_1^{\xi, \eta}(z)$ obtainable from a given number of coefficients ($P^\infty = P + p_\infty$ is fixed, Theorem 3.14) and that the use of additional coefficients (higher $P^\infty = P + p_\infty$) does not worsen $\Phi_{P^\infty,1}^{\xi, \eta}(z)$, cf. (3.65).

Theorems 3.14 and 4.2 are fundamental, for they provide the best estimates of a Stieltjes function $f_1(z)$ over the truncated power series $f_1(z)_x^p$ available at real points and infinity.

3.3 General T-estimates of complex Stieltjes functions.

Now we are able to investigate the problem of an incorporation into estimates of a Stieltjes function $f_1(z)$, among many others, the power series expanded at infinity.

Problem 3.16 *By starting from the $N + 1$ truncated power expansions of $f_1(z)$*

$$f_1(z) = f_1(z)_{\mathbf{x}}^{\mathbf{p}}, \quad (\mathbf{p}) = \begin{pmatrix} p_1, p_2, \dots, p_N, p_\infty \\ x_1, x_2, \dots, x_N, \infty \end{pmatrix} \quad (3.67)$$

let us construct in a complex domain the best bounding function $F_{P+p_\infty,1}(z, u)$ estimating $f_1(z)$.

To solve the Problem 3.16 the parametric power series $f_1^{\xi, \eta}(z)_{\mathbf{x}}^{\mathbf{p}}$ associated with $f_1(z)_{\mathbf{x}}^{\mathbf{p}}$ are needed

$$f_1^{\xi, \eta}(z) = f_1^{\xi, \eta}(z)_{\mathbf{x}}^{\mathbf{p}}, \quad (\mathbf{p}) = \begin{pmatrix} p_1, p_2, \dots, p_N, p_\infty, 1 \\ x_1, x_2, \dots, x_N, \infty, \xi \end{pmatrix}, \quad \text{where } f_1(\xi) = \eta. \quad (3.68)$$

The T -continued fraction expansion of $f_1^{\xi, \eta}(z)$ computed from (3.68) takes the form (see (3.36))

$$f_1^{\xi, \eta}(z) = \mathbf{T}_{P-1}^{(z)} f_P^{\xi, \eta}(z), \quad \text{where } f_P^{\xi, \eta}(\xi) = W_P^{\xi, \eta}(e_P). \quad (3.69)$$

Formula (3.69) leads to the bounding function $F_{P+p_\infty,1}^{\xi, \eta}(z, u)$ given by (cf. (3.58)-(3.60) and (3.69))

$$F_{P+p_\infty,1}^{\xi, \eta}(z, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{F_{1,P}^{\xi, \eta}(z, u, e_P)}{1}, \quad (3.70)$$

$$F_{1,P}^{\xi, \eta}(z, u, e_P) = W_P^{\xi, \eta}(e_P) F_1(z - \xi, u), \quad W_P^{\xi, \eta}(e_P) = (\mathbf{T}_{P-1}^{(\xi)})^{-1} \eta.$$

On account of (3.65)- (3.66), (3.67) and (3.70) we have immediately

$$\begin{aligned} F_{P+p_\infty,1}(z, u) &= \lim_{\xi \rightarrow x} \lim_{\eta \rightarrow \infty} \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{W_P^{\xi, \eta}(e_P) F_1(z - \xi, u)}{1} = \\ &= \lim_{\xi \rightarrow x} \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{W_P^{\xi, \infty}(e_P) F_1(z - x, u)}{1}, \quad (3.71) \\ W_P^{\xi, \infty}(e_P) &= \lim_{\eta \rightarrow \infty} ((\mathbf{T}_{P-1}^{(\xi)})^{-1} \eta), \end{aligned}$$

where (see (3.74))

$$x = \min(x_j, j = 1, 2, \dots, N). \quad (3.72)$$

The bounding function $F_{P+p_\infty,1}(z, u)$ (3.71)-(3.72) solves the Problem 3.16. It is the best estimate of $f_1(z)$ with respect to the given input data (3.67).

3.4 Particular T-estimates of a complex Stieltjes function

Now the particular cases of the bounding functions $F_{P+p_\infty,1}(z, u)$ are studied (cf. (3.71)-(3.72)).

3.4.1 Stieltjes function expanded at zero and infinity

(a) The first term is available only Let the truncated expansions of a Stieltjes function $f_1(z)$ at zero and infinity be given

$$f_1(z)_{\mathbf{x}}^{\mathbf{p}}, \quad (\mathbf{p})_{\mathbf{x}} = \begin{pmatrix} 1, 1 \\ 0, \infty \end{pmatrix}. \quad (3.73)$$

The parametric series $f_1^{\xi, \eta}(z)_{\mathbf{x}}^{\mathbf{p}}$ accompanying (3.73) take the forms

$$f_1^{\xi, \eta}(z)_{\mathbf{x}}^{\mathbf{p}}, \quad (\mathbf{p})_{\mathbf{x}} = \begin{pmatrix} 1, 1, 1 \\ 0, \infty, \xi \end{pmatrix} \quad (3.74)$$

or explicitly

$$\begin{aligned} f_1^{\xi, \eta}(z)_0^1 &= g_1 + O(z), \quad f_1^{\xi, \eta}(z)_\infty^1 = \frac{1}{z} \left(\frac{g_1}{e_2} + O\left(\frac{1}{z}\right) \right), \\ f_1^{-\xi, \eta}(z)_\xi^1 &= \eta + O(x - \xi), \quad \xi < 0, \quad g_1 \leq \eta. \end{aligned} \quad (3.75)$$

The bounding function $F_{2+1,1}^{\xi, \eta}(z, u)$ is given by (cf. (3.75) and (3.70))

$$F_{2+1,1}^{\xi, \eta}(z, u) = \frac{g_1}{1 + z \left(e_2 + F_{1,2}^{\xi, \eta}(z, u, e_2) \right)}, \quad F_{1,2}^{\xi, \eta}(z, u) = W_2^{\xi, \eta}(e_2) F_1(z - \xi, u). \quad (3.76)$$

Relations (3.71), (3.72) and (3.76) yield

$$\frac{g_1}{1 + \xi w_2^{\xi, \infty}} = \infty, \quad w_2^{\xi, \infty} = -\frac{1}{\xi}, \quad F_{2+1,1}^{0, \infty}(z, u) = g_1 F_2(z, u, e_2). \quad (3.77)$$

Here

$$F_2(z, u, e_2) = \lim_{\xi \rightarrow 0} \left(\frac{1}{1 + z e_2 + z \left(\frac{1}{-\xi} - e_2 \right) F_1(z, u)} \right) \quad (3.78)$$

and finally

$$F_2(z, u, e_2) = \begin{cases} \frac{-u}{1 - z e_2 u + (z - 1)(1 + u)} & \text{if } -1 \leq u \leq 0, \\ \frac{u}{1 + z e_2 u} & \text{if } 0 \leq u \leq 1. \end{cases} \quad (3.79)$$

The inclusion regions $\Phi_2^{e_2}(z)$ generated by $F_2(z, u, e_2)$ are depicted in Fig. 3.1, cf. (3.61). From (3.78) and (3.79) the identity follows

$$\lim_{r \rightarrow \infty} \left(\frac{1}{1 + (z - x) (e_P + (r - e_P) F_1(z - x, u))} \right) = F_2(z - x, u, e_P). \quad (3.80)$$

The relation (3.80) will be used to simplify the last terms of T -continued fraction expansions of Stieltjes functions $f_1(z)$.

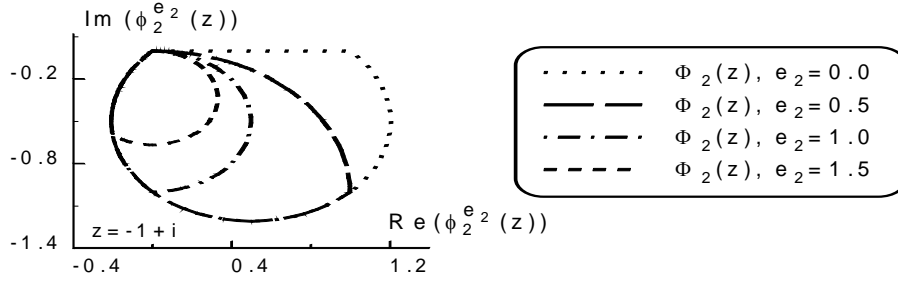


Fig. 3.1 The sequences of the complex boundaries $\phi_2^{e_2}(z)$ and inclusion regions $\Phi_2^{e_2}(z)$ computed from the truncated power series (3.75).

3.4.2 Stieltjes function expanded at a number of real points and infinity

(b) **The case $\xi < x_N = \min(x_j, j = 1, 2, \dots, N)$** Let us estimate $f_1(z)$ from the input data given by

$$f_1(z)_{\mathbf{x}}, (\mathbf{p}) = \left(\begin{matrix} p_1, p_2, \dots, p_N, p_\infty \\ x_1, x_2, \dots, x_N, \infty \end{matrix} \right). \quad (3.81)$$

The parametric power series $f_1^{\xi, \eta}(z)_{\mathbf{x}}^{\mathbf{p}}$ associated with (3.81) is of the form

$$f_1^{\xi, \eta}(z)_{\mathbf{x}}, (\mathbf{p}) = \left(\begin{matrix} p_1, p_2, \dots, p_N, p_\infty, 1 \\ x_1, x_2, \dots, x_N, \infty, \xi \end{matrix} \right). \quad (3.82)$$

From (3.71)-(3.72) and (3.82) we obtain

$$F_{P+p_\infty, 1}(z, u) = \lim_{\xi \rightarrow x_N} \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{F_{1,P}(z, u, e_P)}{1}, \quad (3.83)$$

$$F_{1,P}(z, u, e_P) = W_P^{\xi, \infty}(e_P) F_1(z - x_N, u),$$

where

$$W_P^{\xi, \infty}(e_P) = \lim_{\eta \rightarrow \infty} ((\mathbf{T}_{P-1}^{(\xi)})^{-1} \eta), \quad x = x_N, \quad (3.84)$$

or more precisely

$$\begin{aligned} & F_{P+p_\infty, 1}(z, u) = \\ & = \lim_{\xi \rightarrow x_N} \prod_{k=1}^N \mathbf{T}_{P_{k-1}+1}^{P_k - \delta_{kN}} \frac{g_{P_N}}{1 + (z - x_N) \left(e_P + \left(w_P^{\xi, \infty} - e_P \right) F_1(z - x_N, u) \right)}, \end{aligned} \quad (3.85)$$

where

$$\prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k - \delta_{kN}} \frac{g_j}{1 + (\xi - x_k)e_{j+1} + (\xi - x_k)} \times \frac{g_{P_N}}{1 + (\xi - x_N)w_P^{\xi, \infty}} = \infty, \quad (3.86)$$

$$w_P^{\xi, \infty} = W_P^{\xi, \infty} - e_P.$$

Since $\lim_{\xi \rightarrow x_N} \frac{(\xi - x_N)g_{P_N}}{1 + (\xi - x_N)w_P^{\xi, \infty}} \neq 0$ the relation (3.86) yields

$$w_P^{\xi, \infty} = -\frac{1}{\xi - x_N} + C + O(\xi - x_N), \quad C < \infty, \quad \xi < x_N. \quad (3.87)$$

Finally the Eqs (3.80), (3.86)-(3.87) lead to (cf. (3.79))

$$F_{P+p_\infty,1}(z, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k-\delta_{kN}} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{g_{P-1}F_2(z - x_N, u, e_P)}{1}. \quad (3.88)$$

(c) **The case $\xi < \mathbf{x}_1 = \min(\mathbf{x}_j, j = 2, 3, \dots, N)$** Consider once again the initial input data (3.81). The parametric power expansions $f_1^{\xi, \eta}(z)_x^p$ are given by (3.82). From (3.71)-(3.72) we have

$$F_{P+p_\infty,1}(z, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{W_P^{x_1, \infty} F_1(z - x_1, u)}{1}, \quad (3.89)$$

$$W_P^{x_1, \infty} = \lim_{\eta \rightarrow \infty} ((\mathbf{T}_{P-1}^{(\xi)})^{-1} \eta), \quad x = x_1.$$

(d) **The cases $\xi < \mathbf{x}_N = \min(\mathbf{x}_j, j = 1, 2, \dots, N-1)$ and $\xi < \mathbf{x}_1 = \min(\mathbf{x}_j, j = 2, 3, \dots, N)$** Let us turn our attention to the bounding functions $F_{P+p_\infty,1}^{x_N, \infty}(z, u)$ (3.88) and $F_{P+p_\infty,1}^{x_1, \infty}(z, u)$ (3.89) generated by the input data (3.81)

$$F_{P+p_\infty,1}^{x_N, \infty}(z, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k-\delta_{kN}} \frac{g_j^{x_N}}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{g_{P-1}F_2(z - x_N, u, e_P)}{1}, \quad (3.90)$$

$$F_{P+p_\infty,1}^{x_1, \infty}(z, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j^{x_1}}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{W_P^{x_1, \infty} F_1(z - x_1, u)}{1}.$$

It is proved further (see Theorem 3.20) that even though the coefficients $g_j^{x_1}$ and $g_j^{x_N}$ are different, the complex boundaries $\phi_{P+p_\infty,1}^{x_N, \infty}(z)$ and $\phi_{P+p_\infty,1}^{x_1, \infty}(z)$ determined by the bounding functions $F_{P+p_\infty,1}^{x_N, \infty}(z, u)$ and $F_{P+p_\infty,1}^{x_1, \infty}(z, u)$ coincide

$$\begin{aligned} \phi_{P+p_\infty,1}^{x_N, \infty}(z) &= \phi_{P+p_\infty,1}^{x_1, \infty}(z), \\ \phi_{P+p_\infty,1}^{x_N, \infty}(z) &= \{F_{P+p_\infty,1}^{x_N, \infty}(z, u); -1 \leq u \leq 1\}, \\ \phi_{P+p_\infty,1}^{x_1, \infty}(z) &= \{F_{P+p_\infty,1}^{x_1, \infty}(z, u); -1 \leq u \leq 1\}. \end{aligned} \quad (3.91)$$

By way of illustration of the relations (3.91) let us consider the truncated power expansions of $f_1(z)$ given by

$$f_1(z)_{x_1}^1 = 1 + O(z - x_1), \quad f_1(z)_{x_2}^1 = \frac{1}{7} + O(z - x_2), \quad f_1(z)_{x_3}^1 = 1 + O\left(\frac{1}{z}\right), \quad (3.92)$$

$$x_1 = 0, \quad x_2 = 3, \quad x_3 = \infty$$

and

$$f_1(z)_{x_1}^1 = \frac{1}{7} + O(z - x_1), \quad f_1(z)_{x_2}^1 = 1 + O(z - x_2), \quad f_1(z)_{x_3}^1 = 1 + O\left(\frac{1}{z}\right), \quad (3.93)$$

$$x_1 = 3, \quad x_2 = 0, \quad x_3 = \infty.$$

For the cases (3.92) and (3.93) the relations (3.90) reduce to

$$F_{3+1,1}^{x_2,\infty}(z, u) = \frac{\frac{1}{7}}{1 + \frac{1}{7}(z-3) + (z-3)F_{2,2}^{x_2,\infty}(z, u)}, \quad F_{2,2}^{x_2,\infty}(z, u) = \frac{1}{7}F_2(z, u, 0), \quad (3.94)$$

$$F_{3+1,1}^{x_1,\infty}(z, u) = \frac{1}{1 + z + \frac{z}{1 + (z-3)F_{1,3}^{x_1,\infty}(z, u)}}, \quad F_{1,3}^{x_1,\infty}(z, u) = \frac{1}{3}F_1(z, u, 0).$$

Here $F_1(z, u, 0)$ and $F_2(z, u, 0)$ are given by (1.154) and (3.79). For $z = -1+i$ the relations

$$\phi_{3+1,1}^{x_2,\infty}(z) = \{F_{3+1,1}^{x_2,\infty}(z, u); -1 \leq u \leq 1\} \quad (3.95)$$

and

$$\phi_{3+1,1}^{x_1,\infty}(z) = \{F_{3+1,1}^{x_1,\infty}(z, u); -1 \leq u \leq 1\} \quad (3.96)$$

are evaluated and depicted in Fig. (3.2). In spite of the seemingly different structures

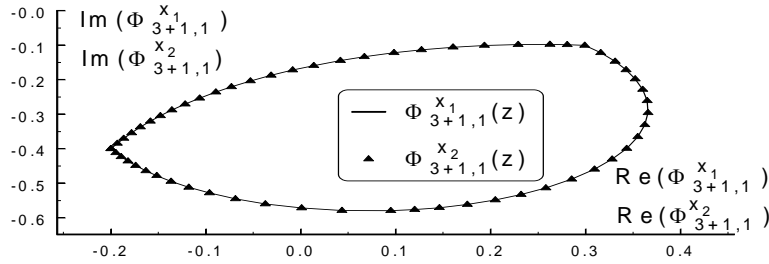


Fig. 3.2 The complex boundaries $\phi_{3+1,1}^{x_1,\infty}(z)$ and $\phi_{3+1,1}^{x_2,\infty}(z, u)$ defined by the bounding functions $F_{3+1,1}^{x_1,\infty}(z, u)$ and $F_{3+1,1}^{x_2,\infty}(z, u)$, cf. (3.94). Note that $\phi_{3+1,1}^{x_1,\infty}(z)$ and $\phi_{3+1,1}^{x_2,\infty}(z, u)$ coincide.

of the T -continued fraction expansions (3.94) the T -boundaries $\phi_{3+1,1}^{x_1,\infty}(z)$ and $\phi_{3+1,1}^{x_2,\infty}(z)$ coincide, cf. Fig. 3.2.

3.4.3 Example

In order to illustrate the TMC FM we consider now the following truncated power expansions

$$\begin{aligned} f_1(z)_{-1}^{+1} &= 0.4694 + O(z+1), \quad f_1(z)_2^1 = 0.18073 + O(z-2), \\ f_1(z)_5^1 &= 0.11527 + O(z-5), \quad f_1(z)_\infty^2 = \frac{1}{z}(1 - 4.0236\frac{1}{z} + O(\frac{1}{z})^2) \end{aligned} \quad (3.97)$$

evaluated from the Stieltjes function

$$f_1(z) = \frac{1}{z} \left(1 + \frac{2.5}{z} \ln \frac{12+z}{20+5z} \right). \quad (3.98)$$

First order estimation The first order bounding function $F_{1+0,1}(z, u)$ generated by $f_1(z)_{-1}^{+1}$ takes the form (cf. (3.97))

$$F_{1+0,1}(z, u) = w_1 F_1(z+1, u), \quad W_1 = f_1(-1) = 0.4694. \quad (3.99)$$

Second order estimation From the expansions $f_1(z)_2^1$ and $f_1(z)_{-1}^{+1}$, it follows

$$F_{2+0,1}(z, u) = \frac{g_1}{1 + (z-2)F_{1,2}(z, u)}, \quad F_{1,2}(z, u, e_2) = W_2(e_2)F_1(z+1, u), \quad (3.100)$$

$$e_2 = 0, \quad g_1 = 0.18073, \quad W_2 = 0.2050.$$

Third order estimation The third order bounding function $F_{2+1,1}(z, u)$ generated by $f_1(z)_2^1$, $f_1(z)_\infty^1$ and $f(z)_{-1}^{+1}$ is equal to

$$F_{2+1,1}(z, u) = \frac{g_1}{1 + (z-2)(e_2 + F_{1,2}(z, u))}, \quad (3.101)$$

$$F_{1,2}(z, u, e_2) = W_2(e_2)F_1(z+1, u),$$

$$g_1 = 0.180733, \quad e_2 = 0.18073, \quad W_2 = 0.02427.$$

Fourth order estimation The expansions $f_1(z)_2^1$, $f_1(z)_5^1$, $f_1(z)_\infty^1$ and $f(z)_{-1}^{+1}$ of $f_1(z)$ yield

$$F_{3+1,1}(z, u) = \frac{g_1}{1 + (z-2)e_2 + \frac{(z-2)g_2}{1 + (z-5)F_{1,3}(z, u, e_3)}}, \quad (3.102)$$

$$F_{1,3}(z, u, e_3) = W_3(e_3)F_1(z+1, u),$$

$$g_1 = 0.180733, \quad e_2 = 0.18073, \quad g_2 = 0.0086, \quad e_3 = 0, \quad W_3 = 0.1078.$$

Fifth order estimation From $f_1(z)_2^1$, $f_1(z)_5^1$, $f_1(z)_\infty^2$ and $f(z)_{-1}^{+1}$, it follows

$$F_{3+2,1}(z, u) = \frac{g_1}{1 + (z-2)e_2 + \frac{(z-2)g_2}{1 + (z-5)e_3 + (z-5)F_{1,3}(z, u, e_3)}}, \quad (3.103)$$

$$F_{1,3}(z, u, e_3) = W_3(e_3)F_1(z+1, u),$$

$$g_1 = 0.180733, \quad e_2 = 0.18073, \quad g_2 = 0.0086, \quad e_3 = 0.0967, \quad W_3 = 0.0111.$$

For $z = -3 + i$ the narrowing lens-shaped estimations (3.100)-(3.103) and the value of the Stieltjes function (3.98) are depicted in Fig. 3.3.

3.5 Multipoint Padé approximants to power expansions of Stieltjes function

Let us consider the multipoint Padé approximants

$$[m_R/n_R]_{\mathbf{x}(x_{N+1})}^{\mathbf{r}(R)}(z), \quad \left(\begin{array}{c} \mathbf{r}(R) \\ \mathbf{x}(x_{N+1}) \end{array} \right) = \left(\begin{array}{c} p_1, p_2, \dots, p_N, p_{N+1} \\ x_1, x_2, \dots, x_N, x_{N+1} \end{array} \right), \quad (3.104)$$

$$[m_R/n_R]_{\mathbf{x}(x_{N+1})}^{\mathbf{r}(R)}(z) = \frac{a_0(x_{N+1}) + a_1(x_{N+1})z^1 + \dots + a_{m_R}(x_{N+1})z^{m_R}}{1 + b_1(x_{N+1})z^1 + b_2(x_{N+1})z^2 + \dots + b_{n_R}(x_{N+1})z^{n_R}}, \quad (3.105)$$

$$m_R = R - 1 - n_R, \quad n_R = E(R/2), \quad P = \sum_{j=1}^N p_j, \quad R = P + p_{N+1}$$

to the Stieltjes functions $f_1(z)$ satisfying the relation (cf. (3.1))

$$\lim_{z \rightarrow \infty} |zf_1(z)| < \infty. \quad (3.106)$$

Definition 3.17 The rational function $[m_R/n_R]_{x(\infty)}^{r(R)}(z)$ defined by

$$\begin{aligned}
 [m_R/n_R]_{x(\infty)}^{r(R)}(z) &= \lim_{x_{N+1} \rightarrow \infty} [m_R/n_R]_{x(x_{N+1})}^{r(R)}(z) = \\
 &= \frac{a_0(\infty) + a_1(\infty)z^1 + a_2(\infty)z^2 + \dots + a_{m_R}(\infty)z^{m_R}}{1 + b_1(\infty)z^1 + b_2(\infty)z^2 + \dots + b_{n_R}(\infty)z^{n_R}}
 \end{aligned}
 \tag{3.107}$$

we call the T -multipoint Padé approximant to $f_1(z)$. If R is odd (even) we call it the odd (even) T -multipoint Padé ones.

From (3.104)-(3.105), it follows that the contiguous odd, even T -multipoint Padé approximants to $f_1(z)$ are of the forms

$$\begin{aligned}
 [m_R/n_R]_{x(\infty)}^{r(R)}(z) &= \frac{a_0(\infty) + a_1(\infty)z^1 + a_2(\infty)z^2 + \dots + a_{m_R}(\infty)z^{m_R}}{1 + b_1(\infty)z^1 + b_2(\infty)z^2 + \dots + b_{n_R}(\infty)z^{m_R}}, \\
 [m_{R-1}/n_{R-1}]_{x(\infty)}^{r(R-1)}(z) &= \frac{a_0(\infty) + a_1(\infty)z^1 + \dots + a_{m_{R-1}}(\infty)z^{m_{R-1}-1}}{1 + b_1(\infty)z^1 + \dots + b_{n_{R-1}}(\infty)z^{m_{R-1}-1}},
 \end{aligned}
 \tag{3.108}$$

respectively. The main properties of $[m_R/n_R]_{x(\infty)}^{r(R)}(z)$ and $[m_{R-1}/n_{R-1}]_{x(\infty)}^{r(R-1)}(z)$ given by (3.108) state the following theorem:

Theorem 3.18 Since for R odd the coefficient $a_{m_R}(\infty)$ appearing in (3.108₁) vanishes

$$a_{m_R}(\infty) = 0 \tag{3.109}$$

the contiguous odd (3.108₁) and even (3.108₂) T -multipoint Padé approximants coincide

$$[m_R/n_R]_{x_1, x_2, \dots, x_N, \infty}^{p_1, p_2, \dots, p_N, p_\infty}(z) = [m_{R-1}/n_{R-1}]_{x_1, x_2, \dots, x_N, \infty}^{p_1, p_2, \dots, p_N, p_\infty-1}(z). \tag{3.110}$$

Proof. If $x_{N+1} \neq 0$ and $|z - x_{N+1}| \rightarrow 0$ it follows from (2.121) and (3.106) that

$$zf_1(z) - z[m_R/n_R]_{x(x_{N+1})}^{r(R)}(z) = zO((z - x_{N+1})^{p_{N+1}}) = O\left(\left(\frac{1}{z} - \frac{1}{x_{N+1}}\right)^{p_{N+1}}\right). \tag{3.111}$$

By substituting $z = 1/s$ in 3.111) we obtain at once

$$\varphi_1(s) - \frac{1}{s}[m_R/n_R]_{y(s_{N+1})}^{r(R)}(1/s) = O((s - s_{N+1})^{p_{N+1}}), \quad \varphi_1(s) = \frac{1}{s}f_1\left(\frac{1}{s}\right). \tag{3.112}$$

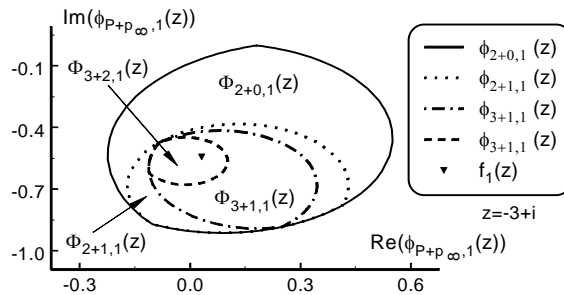


Fig. 3.3 The complex boundaries $\phi_{P+p_{\infty,1}}(z)$ evaluated from the truncated power series (3.100)-(3.103) representing the Stieltjes function (3.98).

For R odd the relation (3.108₁) and (3.112) yield

$$\varphi_1(s) - \frac{1}{s} \left(\frac{a_0(x_{N+1})s^{m_R} + \cdots + a_{m_R}(x_{N+1})}{s^{m_R} + b_1(x_{N+1})s^{m_R-1} + \cdots + b_{m_R}(x_{N+1})} \right) = O((s - s_{N+1})^{p_{N+1}}). \quad (3.113)$$

Hence the following equality holds

$$\varphi_1(s_{N+1}) = \frac{1}{s_{N+1}} \left(\frac{(s_{N+1})^{m_R} a_0(x_{N+1}) + \cdots + a_{m_R}(x_{N+1})}{(s_{N+1})^{m_R} + (s_{N+1})^{m_R-1} b_1(x_{N+1}) + \cdots + b_{m_R}(x_{N+1})} \right). \quad (3.114)$$

On account of (3.106) we have

$$\lim_{x_{N+1} \rightarrow \infty} \varphi_1(s_{N+1}) < \infty, \quad s_{N+1} = \frac{1}{x_{N+1}}. \quad (3.115)$$

Thus from (3.114), it follows

$$\lim_{x_{N+1} \rightarrow \infty} a_{m_R}(x_{N+1}) = a_{m_R}(\infty) = 0, \quad \varphi_1(0) = \frac{a_{m_R-1}(\infty)}{b_{m_R}(\infty)}. \quad (3.116)$$

The Eqs (3.108₁) and (3.116) yield

$$[m_R/n_R]_{\mathbf{x}(\infty)}^{\mathbf{r}(R)}(z) = \frac{a_0(\infty) + \cdots + a_{m_R-1}(\infty)z^{m_R-1}}{1 + b_1(\infty)z^1 + \cdots + b_{m_R}(\infty)z^{m_R}} = [m_{R-1}/n_{R-1}]_{\mathbf{x}(\infty)}^{\mathbf{r}(R-1)}(z). \quad (3.117)$$

The relation (3.117) and (3.110) coincide. The proof is complete. ■

As an illustration of the Definition 3.17 and the Theorem 3.18 let us compute the multipoint Padé approximants to the truncated power expansions

$$f_1(z)_{\mathbf{x}}, \quad (\mathbf{r}) = \begin{pmatrix} +1, 2 \\ -1, \infty \end{pmatrix} \quad (3.118)$$

of a Stieltjes function

$$f_1(z) = \frac{1}{z} \left(1 + \frac{25}{10z} \ln \frac{12+z}{20+5z} \right). \quad (3.119)$$

From (3.118), it follows

$$R = 1 + 2 = 3, \quad n_3 = E(3/2) = 1, \quad m_3 = 3 - 1 - 1 = 1. \quad (3.120)$$

The equation (3.105) reduces to

$$[1/1]_{-1, \infty}^{+1, 2}(z) = \lim_{x_2 \rightarrow \infty} [1/1]_{-1, x_2}^{+1, 2}(z), \quad (3.121)$$

where

$$[1/1]_{-1, x_2}^{+1, 2}(z) = \frac{a_0(x_2) + a_1(x_2)z}{1 + b_1(x_2)z}. \quad (3.122)$$

On the basis of (2.121) one obtains

$$f_1(z)_{-1}^{+1} - [1/1]_{-1, x_2}^{+1, 2}(z) = O((z+1)), \quad (3.123)$$

$$\frac{1}{s} f_1\left(\frac{1}{s}\right) - \frac{1}{s} [1/1]_{-1, s_2}^{+1, 2}\left(\frac{1}{s}\right) = O(s^2), \quad s = \frac{1}{z}, \quad s_2 = \frac{1}{z_2}.$$

For $s_2 \rightarrow 0$ the substitutions (3.122) and (3.119) into (3.123) yield

$$\frac{a_0 - a_1}{1 - b_1} = 0.4695, \quad 1 = \frac{s_2 a_0 + a_1}{(s_2 + b_1) s_2}, \quad 4.0236 = \frac{2a_1 s_2 + a_0 s_2^2 + a_1 b_1}{s_2^2 (s_2 + b_1)^2} \quad (3.124)$$

and for $s_2 = 0$

$$\frac{a_0 - a_1}{1 - b_1} = 0.4695, \quad \frac{a_0}{b_1} = 1, \quad a_1 b_1 = 0. \quad (3.125)$$

Finally we get

$$a_1 = 0, \quad a_0 = 0.3195, \quad b_1 = 0.3195. \quad (3.126)$$

From (3.121)-(3.122), it follows

$$[1/1]_{-1, \infty}^{+1, 2}(z) = \frac{0.3195}{1 + 0.3195z} = [0/1]_{-1, \infty}^{+1, 1}(z). \quad (3.127)$$

Note that the results (3.126₁) and (3.127) confirm the equalities (3.110).

Now we interrelate the bounding functions $F_{P+p_\infty, 1}(z, u)$ with the Padé approximants $[m_R/n_R]_{x_1, x_2, \dots, x_N, \infty, \xi}^{p_1, p_2, \dots, p_N, p_\infty, 1}(z)$ and $[m_{R-1}/n_{R-1}]_{x_1, x_2, \dots, x_N, \infty, \xi}^{p_1, p_2, \dots, p_N, p_\infty, 0}(z)$.

Corollary 3.19 *The bounding functions $F_{P+p_\infty, 1}(z, u)$ given by*

$$F_{P+p_\infty, 1}(z, u) = \bigvee_{k=1}^N \mathbf{T}_{P_{k-1}+1}^{P_k} F_{1, P}(z, u), \quad u = -1, 1, \quad (3.128)$$

$$F_{P+p_\infty, 1}(z, u) = \bigvee_{k=1}^N \mathbf{T}_{P_{k-1}+1}^{P_k} F_{1, P}(z, u), \quad u = 0$$

and the T -multipoint Padé approximants

$$[m_R/n_R]_{\mathbf{x}}^{r(R)}(z), \quad \begin{pmatrix} r(R) \\ \mathbf{x} \end{pmatrix} = \begin{pmatrix} p_1, p_2, \dots, p_N, p_\infty, 1 \\ x_1, x_2, \dots, x_N, \infty, \xi \end{pmatrix}, \quad (3.129)$$

$$[m_{R-1}/n_{R-1}]_{\mathbf{x}}^{r(R-1)}(z), \quad \begin{pmatrix} r(R-1) \\ \mathbf{x} \end{pmatrix} = \begin{pmatrix} p_1, p_2, \dots, p_N, p_\infty, 0 \\ x_1, x_2, \dots, x_N, \infty, \xi \end{pmatrix}$$

coincide, i.e.

$$F_{P+p_\infty, 1}(z, -1) = F_{P+p_\infty, 1}(z, 1) = [m_{R-1}/n_{R-1}]_{x_1, x_2, \dots, x_N, \infty, \xi}^{p_1, p_2, \dots, p_N, p_\infty, 0}(z), \quad (3.130)$$

$$F_{P+p_\infty, 1}(z, 0) = [m_R/n_R]_{x_1, x_2, \dots, x_N, \infty, \xi}^{p_1, p_2, \dots, p_N, p_\infty, 1}(z).$$

Proof. From Definition 3.17 and Theorem 3.11, it follows the identities (3.130) ■
In order to illustrate the Corollary (3.19) we consider the truncated power expansions

$$f_1(z)_{-1}^{+1} = \eta + O(z - \xi), \quad \xi = -1, \quad \eta = 0.4694; \quad f_1(z)_2^1 = 0.18073 + O(z); \quad (3.131)$$

$$f_1(z)_5^1 = 0.11527 + O(z - 3); \quad z f_1(z)_\infty^2 = 1 - 4.0236 \frac{1}{z} + O\left(\frac{1}{z}\right)^2$$

of the Stieltjes function

$$f_1(z) = \frac{1}{z} \left(1 + \frac{2.5}{z} \ln \frac{1.2 + 0.1z}{2 + 0.5z} \right). \quad (3.132)$$

The bounding functions $F_{3+1,1}(z, u)$ and $F_{3+2,1}(z, u)$ evaluated from (3.131) are of the forms (cf. (3.103))

$$F_{3+1,1}(z, u) = \frac{0.181}{1 + 0.181(z - 2) + \frac{0.009(z - 2)}{1 + W_3(e_3)(z - 5)F_{1,3}(z, u, 0)}}, \quad (3.133)$$

$$F_{1,3}(z, u, e_3) = W_3(e_3)F_1(z + 1, u), \quad W_3(e_3) = 0.1078, \quad e_3 = 0,$$

$$F_{3+2,1}(z, u) = \frac{0.181}{1 + 0.181(z - 2) + \frac{0.009(z - 2)}{1 + e_3(z - 5) + (z - 5)F_{1,3}(z, u, e_3)}}, \quad (3.134)$$

$$F_{1,3}(z, u, e_3) = W_3(e_3)F_1(z + 1, u), \quad W_3(e_3) = 0.011, \quad e_3 = 0.097.$$

By substituting

$$F_{1,3}(z, 0, 0) = 0.1078, \quad F_{1,3}(z, 0, 0.097) = 0, 011 \quad (3.135)$$

into (3.134) we obtain

$$F_{3+1,1}(z, 0) = [2/2]_{2,5,\infty,-1}^{1,1,1,+1}(z) = \frac{0.300 + 0.0703z}{1.000 + 0.580z + 0.070z^2}, \quad (3.136)$$

$$F_{3+2,1}(z, 0) = [1/2]_{2,5,\infty,-1}^{1,1,2,+1}(z) = \frac{0.300 + 0.0703z}{1.000 + 0.580z + 0.070z^2}. \quad (3.137)$$

Note that the contiguous odd and even T -Padé approximants $[2/2]_{2,5,\infty,-1}^{1,1,2,+1}(z)$ and $[1/2]_{2,5,\infty,-1}^{1,1,1,+1}(z)$ to the Stieltjes function (3.132) coincide, cf. Theorem 3.18.

3.5.1 T -inclusions regions generated by T -multipoint Padé approximants

Consider the following functions

$$F_{P+p_\infty,1}(z, u), \quad u \in [-1, 0]; \quad F_{P+p_\infty,1}(z, u), \quad u \in [0, 1] \quad (3.138)$$

and

$$F_{P+1+p_\infty,1}(z, u), \quad u \in [-1, 0]; \quad F_{P+1+p_\infty,1}(z, u), \quad u \in [0, 1] \quad (3.139)$$

forming the contiguous bounding ones

$$F_{P+p_\infty,1}(z, u), \quad u \in [-1, 1] \quad \text{and} \quad F_{P+1+p_\infty,1}(z, u), \quad u \in [-1, 1]. \quad (3.140)$$

The functions 3.140 estimate $f_1(z)$, where (cf. (3.60))

$$F_{P+p_\infty,1}(z, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{F_{1,P}(z, u, e_P)}{1}, \quad (3.141)$$

$$F_{1,P}(z, u, e_P) = W_P(e_P)F_1(z - \xi, u)$$

and

$$F_{P+1+p_\infty,1}(z, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{F_{1,P+1}(z, u, 0)}{1}, \quad (3.142)$$

$$F_{1,P+1}(z, u, 0) = W_{P+1}(0)F_1(z - \xi, u).$$

In addition the relations are true

$$\begin{aligned} F_{1,P}(z, -1) = F_{1,P}(z, 1) = F_{1,P+1}(z, -1) = F_{1,P+1}(z, 1) = 0, \\ F_{1,P}(z, 0, e_P) = W_P(e_P), \quad F_{1,P+1}(z, 0, 0) = W_{P+1}(0). \end{aligned} \quad (3.143)$$

Since

$$F_{P+1+p_\infty,1}(\xi, 0) = F_{P+p_\infty,1}(\xi, 0) \quad (3.144)$$

then

$$F_{1,P}(\xi, 0) = \frac{g_P}{1 + (\xi - x_N)F_{1,P+1}(\xi, 0)}. \quad (3.145)$$

From (3.143)-(3.145), it follows

$$W_{P+1} = \frac{g_P - W_P}{W_P(\xi - x_N)}. \quad (3.146)$$

According to Conclusion 2.13 the new curve (3.140₂) touches the old one (3.140₁) at two points $F_{P+1+p_\infty,1}(z, 1)$ and $F_{P+1+p_\infty,1}(z, 0)$. On account of that the parametric multipoint Padé approximants $H_{P+1+p_\infty,1}(z, g_P)$ depending on the coefficient g_P (cf. (3.141), (3.142) and (3.146))

$$H_{P+1+p_\infty,1}(z, g_P) = \begin{cases} F_{P+1+p_\infty,1}(z, 1, -g_P) & \text{if } -w_P \leq g_P \leq 0, \\ F_{P+1+p_\infty,1}(z, 0, g_P) & \text{if } 0 \leq g_P \leq w_P, \end{cases} \quad (3.147)$$

$$F_{P+1+p_\infty,1}(z, 1, -g_P) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)} \times \frac{-g_P}{1}, \quad (3.148)$$

$$F_{P+1+p_\infty,1}(z, 0, g_P) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)} \times \frac{g_P}{1 + (z - x_N) \frac{g_P - W_P}{W_P(\xi - x_N)}},$$

coincide with (3.138₁) and (3.138₂), respectively, i.e.

$$\begin{aligned} \chi_{P+1+p_\infty,1}(z) &= \phi_{P+p_\infty,1}(z), \\ \chi_{P+1+p_\infty,1}(z) &= \{w \in \mathbb{C} : w = H_{P+1+p_\infty,1}(z, g_P); g_P \in [-w_P, w_P]\}, \\ \phi_{P+p_\infty,1}(z) &= \{w \in \mathbb{C} : w = F_{P+p_\infty,1}(z, u); u \in [-1, 1]\}. \end{aligned} \quad (3.149)$$

To illustrate the identities (3.149) we consider the truncated power expansions

$$\begin{aligned} f_1(z)_{-1}^{+1} &= \eta + O(z - \xi), \quad \xi = -1; \quad \eta = 0.4694; \quad f_1(z)_{-2}^{\frac{1}{2}} = 0.18073 + O(z - 2); \\ f_1(z)_{-5}^{\frac{1}{5}} &= 0.11527 + O(z - 5); \quad z f_1(z)_{\infty}^2 = 1 - 4.0236 \frac{1}{z} + O\left(\frac{1}{z}\right)^2 \end{aligned} \quad (3.150)$$

computed from the Stieltjes function

$$f_1(z) = \frac{1}{z} \left(1 + \frac{2.5}{z} \ln \frac{1.2 + 0.1z}{2 + 0.5z} \right). \quad (3.151)$$

For the input data (3.150)-(3.151) the bounding functions $F_{P+p_\infty,1}(z, u)$ and $H_{P+1+p_\infty,1}(z, g_P)$ are evaluated. The boundaries $\phi_{P+p_\infty,1}(z)$ and $\chi_{P+1+p_\infty,1}(z)$ generated by $F_{P+p_\infty,1}(z, u)$ and $H_{P+1+p_\infty,1}(z, g_P)$ are depicted in Fig. 3.4.

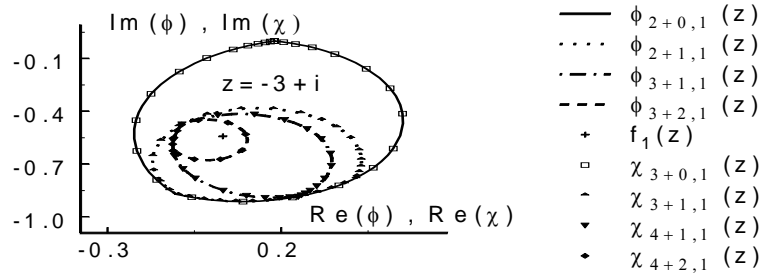


Fig. 3.4 The complex boundaries $\chi_{P+1+p_\infty,1}(z)$ and $\phi_{P+p_\infty,1}(z)$ defined by the bounding functions $H_{P+1+p_\infty,1}(z, g_P)$, $0 \leq g_P \leq w_P$ and $F_{P+p_\infty,1}(z, u)$, $-1 \leq u \leq 1$, computed from the truncated power series (3.150). Note that $\chi_{P+1+p_\infty,1}(z)$ and $\phi_{P+p_\infty,1}(z)$ coincide.

Theorem 3.20 Let $F_{P+p_\infty,1}(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_1, x_2, \dots, x_N, \infty, \xi}, u)$ be a bounding function evaluated from the truncated power series of Stieltjes $f_1(z)^{p_1, \dots, p_N, p_\infty, 1}_{x_1, \dots, x_N, \infty, \xi}$. For all permutations $(\alpha_1, \dots, \alpha_N)$ of natural numbers $(1, 2, \dots, N)$ the inclusion regions

$$\Phi_{P+p_\infty,1}(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_1, x_2, \dots, x_N, \infty, \xi}) \text{ and } \Phi_{P+p_\infty,1}(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi}) \quad (3.152)$$

generated by the bounding functions

$$F_{P+p_\infty,1}(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_1, x_2, \dots, x_N, \infty, \xi}, u) \text{ and } F_{P+p_\infty,1}(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi}, 1) \quad (3.153)$$

coincide, i.e.

$$\Phi_{P+p_\infty,1}(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_1, x_2, \dots, x_N, \infty, \xi}) = \Phi_{P+p_\infty,1}(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi}). \quad (3.154)$$

Proof. For a fixed permutation of $(\alpha_1, \alpha_2, \dots, \alpha_N)$ the following sets of three points

$$\left| \begin{array}{c} F_{P+p_\infty,1} \left(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi}, 1 \right) \\ F_{P+1+p_\infty,1} \left(z, \frac{p_1, p_2, \dots, p_{N+1}, p_\infty, 1}{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi}, 0 \right) \\ F_{P+p_\infty,1} \left(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi}, 0 \right) \end{array} \right| \quad (3.155)$$

and

$$\left| \begin{array}{c} F_{P+p_\infty,1} \left(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi}, 1 \right) \\ F_{P+1+p_\infty,1} \left(z, \frac{p_1, p_2, \dots, p_{N+1}, p_\infty, 1}{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi}, 1 \right) \\ F_{P+p_\infty,1} \left(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi}, 0 \right) \end{array} \right|. \quad (3.156)$$

generate the complex boundaries $\Phi_{P+p_\infty,1} \left(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi} \right)$. Since the multipoint continued fractions (3.155) and (3.156) are the Padé approximants to $f_1(z)$ we have (cf. Theorem 3.13)

$$F_{P+p_\infty,1} \left(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_1, x_2, \dots, x_N, \infty, \xi}, j \right) = F_{P+p_\infty,1} \left(z, \frac{p_1, p_2, \dots, p_N, p_\infty, 1}{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi}, j \right), \quad (3.157)$$

$$F_{P+1+p_\infty,1} \left(z, \frac{p_1, p_2, \dots, p_{N+1}, p_\infty, 1}{x_1, x_2, \dots, x_N, \infty, \xi}, j \right) = F_{P+1+p_\infty,1} \left(z, \frac{p_1, p_2, \dots, p_{N+1}, p_\infty, 1}{x_{\alpha_1}, x_{\alpha_2}, \dots, x_{\alpha_N}, \infty, \xi}, j \right),$$

where $j = 0, 1$. The relations (3.157) imply the equality (3.154). ■

3.6 Fundamental inequalities for T-multipoint Padé approximants to Stieltjes functions

For $z = x \in \mathbb{R}$ the lens-shaped inclusion region $\Phi_{P+p_\infty,1}(z)$ (3.61) and the complex boundary $\phi_{P+p_\infty,1}(z)$ of $\Phi_{P+p_\infty,1}(z)$ (3.62) reduce to the segment lying on the real axis

$$\begin{aligned} \Phi_{P+p_\infty,1}(x) = \phi_{P+p_\infty,1}(x) &= \{w \in \mathbb{R} : w = F_{P+p_\infty,1}(x, u); -1 \leq u \leq 0\}, \\ f_1(x) &\in \Phi_{P+p_\infty,1}(x), \end{aligned} \quad (3.158)$$

where

$$F_{P+p_\infty,1}(x, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (x - x_k)e_{j+1}} \times \frac{F_{1,P}(x, u, e_p)}{1}, \quad \xi < x, \quad (3.159)$$

$$F_{1,P}(x, u, e_p) = W_p(e_p)F_1(x - \xi, u), \quad F_1(x, u) = (1 + u), \quad -1 \leq u \leq 0.$$

It is convenient to represent $F_{P+p_\infty,1}(x, u)$ (3.159) as follows

$$\begin{aligned} F_{P+p_\infty,1}(x, u) &= \frac{g_1}{1 + (x - x_1)e_2 + (x - x_1)F_{P-1,2}(x, u)}, \\ F_{P-1,2}(x, u) &= \frac{g_2}{1 + (x - x_1)e_3 + (x - x_1)F_{P-2,3}(x, u)}, \\ &\dots, \\ F_{2,P-1}(x, u) &= \frac{g_{P-1}}{1 + (x - x_N)e_P + (x - x_N)F_{1,P}(x, u)}, \quad F_{1,P}(x, u) = \\ &W_P(e_P)F_1(x - \xi, u), \quad F_1(x - \xi, u) = (1 + u), \quad -1 \leq u \leq 0, \quad \xi < x < \infty. \end{aligned} \quad (3.160)$$

Hence we have

$$\begin{aligned} \frac{\partial F_{P+p_\infty,1}(x, u)}{\partial u} &= -\frac{g_1(x - x_1)}{(1 + (x - x_1)(e_2 + F_{P-1,2}(x, u)))^2} \frac{\partial F_{P-1,2}(x, u)}{\partial u}, \\ \frac{\partial F_{P-1,2}(x, u)}{\partial u} &= -\frac{g_2(x - x_1)}{(1 + (x - x_1)(e_3 + F_{P-2,3}(x, u)))^2} \frac{\partial F_{P-2,3}(x, u)}{\partial u}, \\ &\dots, \\ \frac{\partial F_{2,P-1}(x, u)}{\partial u} &= -\frac{g_{P-1}(x - x_N)}{(1 + (x - x_N)(e_P + F_{1,P}(x, u, e_P)))^2} \frac{F_{1,P}(x, u)}{\partial u}. \end{aligned} \quad (3.161)$$

Further simplification of (3.161) yields

$$\frac{\partial F_{P+p_\infty,1}(x, u)}{\partial u} = W_P \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \left(\frac{-g_j(x - x_k)}{(1 + (x - x_k)(e_{j+1} + F_{P-j,1+j}(x, u)))^2} \right), \quad (3.162)$$

where

$$W_P = w_P - e_P. \quad (3.163)$$

Thus

$$\text{sign} \left(\frac{\partial F_{P+p_\infty,1}(x, u)}{\partial u} \right) = \text{sign} \left(\prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} (x_k - x) \right), \quad \xi \leq x < \infty, \quad (3.164)$$

or more exactly

$$\text{sign} \left(\frac{\partial F_{P+p_\infty,1}(x, u)}{\partial u} \right) = \text{sign} \left((x_1 - x)^{P_1} (x_2 - x)^{P_2} \dots (x_N - x)^{P_N} \right). \tag{3.165}$$

Relation (3.165) means

$$\text{sign} \left(\frac{\partial F_{P+p_\infty,1}(x, u)}{\partial u} \right) = \begin{cases} (-1)^0 & \text{if } \xi < x < x_1, \\ (-1)^{P_1} & \text{if } x_1 < x < x_2, \\ (-1)^{P_2} & \text{if } x_2 < x < x_3, \\ \dots & \dots \\ (-1)^{P_N} & \text{if } x_N < x < \infty. \end{cases} \tag{3.166}$$

The bounding function $F_{P+p_\infty,1}(x, u)$ is monotonic with respect to u . Hence

$$\begin{aligned} (-1)^0 F_{P+p_\infty,1}(x, -1) &\leq (-1)^{P_0} f_1(x) && \text{if } \xi < x \leq x_1, \\ (-1)^{P_1} F_{P+p_\infty,1}(x, -1) &\leq (-1)^{P_1} f_1(x) && \text{if } x_1 \leq x \leq x_2, \\ (-1)^{P_2} F_{P+p_\infty,1}(x, -1) &\leq (-1)^{P_2} f_1(x) && \text{if } x_2 \leq x \leq x_3, \\ \dots &\dots && \dots \\ (-1)^{P_N} F_{P+p_\infty,1}(x, -1) &\leq (-1)^{P_N} f_1(x) && \text{if } x_N \leq x < \infty \end{aligned} \tag{3.167}$$

and

$$\begin{aligned} (-1)^0 F_{P+p_\infty,1}(x, 0) &\leq (-1)^{P_0+1} f_1(x) && \text{if } \xi < x \leq x_1, \\ (-1)^{P_1} F_{P+p_\infty,1}(x, 0) &\leq (-1)^{P_1+1} f_1(x) && \text{if } x_1 \leq x \leq x_2, \\ (-1)^{P_2} F_{P+p_\infty,1}(x, 0) &\leq (-1)^{P_2+1} f_1(x) && \text{if } x_2 \leq x \leq x_3, \\ \dots &\dots && \dots \\ = (-1)^{P_N} F_{P+p_\infty,1}(x, 0) &\leq (-1)^{P_N+1} f_1(x) && \text{if } x_N \leq x < \infty, \end{aligned} \tag{3.168}$$

where $P_j, j = 1, 2, \dots, N$ and P are given by (2.14).

Theorem 3.21 Consider the non-decreasing power series of Stieltjes

$$f_1(x) = \sum_{i=0}^{p_j} c_{ij}(x - x_j)^i + O((x - x_j)^{p_j}), \quad j = 1, \dots, N, \tag{3.169}$$

$$f_1(x) = \frac{1}{x} \sum_{i=0}^{p_\infty} d_{i\infty} \left(\frac{1}{x} \right)^i + O \left(\left(\frac{1}{x} \right)^{p_j} \right), \quad f_1(x) = \eta + O(x - \xi)$$

and accompanying them the $L_{P+p_\infty}(x)$ characteristic functions (2.6). For fixed ξ and η the multipoint Padé approximants $F_{P+p_\infty,1}(x, J), x \in \mathbb{R} \setminus [-\infty, \xi]$ to the power expansions (3.169), where $J = 0, 1$, satisfy the following inequalities

$$\begin{aligned} (-1)^{L_{P+p_\infty-1}(x)} F_{P+p_\infty-1,1}(x, 0) &\leq (-1)^{L_{P+p_\infty-1}(x)} F_{P+p_\infty,1}(x, 0), \\ (-1)^{L_{P+p_\infty-1}(x)} F_{P+p_\infty-1,1}(x, -1) &\geq (-1)^{L_{P+p_\infty-1}(x)} F_{P+p_\infty-1,1}(x, -1), \\ (-1)^{L_{P+p_\infty}(x)} F_{P+p_\infty,1}(x, 0) &\leq (-1)^{L_{P+p_\infty}(x)} f_1(x) \leq \\ &(-1)^{L_{P+p_\infty}(x)} F_{P+p_\infty,1}(x, -1). \end{aligned} \tag{3.170}$$

Proof. The inequalities (3.170) are direct consequence of the relations (3.167) and (3.168). ■

From (3.170) and Theorem 3.14, it follows that the Padé approximants $F_{P+p_\infty,1}(x, J)$, $J = 0, -1$ form the optimum upper and lower bounds on $f_1(x)$ obtainable using only the given number of coefficients and that the use of additional coefficients (higher $(P + p_\infty)$) does not worsen the bounds $F_{P+p_\infty,1}(x, J)$, $J = 0, -1$ on $f_1(x)$.

The Theorems 3.14 and 3.21 are fundamental, for they provide the best upper and lower bounds on $f_1(x)$ obtainable from the truncated power series of Stieltjes $f_1(x)_x^p$. If the power expansion of $f_1(x)$ at infinity is not available the T - estimates of $f_1(x)$ (3.170) reduce to the S -estimates of $f_1(x)$, cf. (2.172). Hence the inequalities for T -multipoint Padé approximants (3.170) generalize the corresponding S -inequalities (2.172).

3.7 Particular cases of the optimum T-estimates of a Stieltjes function in a real domain.

The particular cases of the general estimates $F_{P+p_\infty,1}(x, 0)$ and $F_{P+p_\infty,1}(x, -1)$ of $f_1(x)$ will be investigated, cf. (3.170).

3.7.1 Stieltjes function expanded at zero and infinity

(a) The first terms are available only Let the truncated expansions of a Stieltjes function $f_1(x)$ at zero and infinity be given

$$f_1(x)_x^r, \binom{r}{x} = \binom{1,1}{0,\infty}. \quad (3.171)$$

The parametric power series $f_1^{\xi,\eta}(x)_x^p$ accompanying (3.171) take the forms (cf. Theorem (4.2))

$$f_1^{\xi,\eta}(x)_x^r, \binom{r}{x} = \binom{1,1,1}{0,\infty,\xi}. \quad (3.172)$$

From (3.172), it follows

$$f_1^{\xi,\eta}(x)_0^1 = g_1 + O(x - 0), \quad f_1^{\xi,\eta}(x)_\infty^2 = \frac{1}{x} \left(\frac{g_1}{e_2} + O\left(\frac{1}{x}\right) \right), \quad (3.173)$$

$$f_1^{\xi,\eta}(x)_\xi^1 = \eta + O(x - \xi), \quad \xi < 0, \quad g_1 \leq \eta.$$

The input data (3.173) generates the characteristic function $L_{2+1}(x)$ (cf. (2.6))

$$L_{2+1}(x) = 2H(x), \quad \xi < x < \infty \quad (3.174)$$

and the bounding one (cf. (3.78))

$$F_{2+1,1}^{0,\infty}(x, u) = g_1 F_2(x, u, e_2), \quad (3.175)$$

where on account of (3.79₂)

$$F_{2+1,1}(x, u) = \frac{u}{1 + x e_2 u}, \quad 0 \leq u \leq 1. \quad (3.176)$$

The Padé approximants $F_{2+1,1}^{0,\infty}(x, 0)$ and $F_{2+1,1}^{0,\infty}(x, 1)$ defined by (3.175)-(3.176) satisfy the inequalities (3.170)

$$(-1)^{2H(x)} F_{2+1,1}^{0,\infty}(x, 0) \leq (-1)^{2H(x)} f_1(x) \leq (-1)^{2H(x)} F_{2+1,1}^{0,\infty}(x, 1). \quad (3.177)$$

By substituting the relations (3.175) and (3.176) into (3.177) we arrive at

$$0 \leq f_1(x) \leq \frac{g_1}{1 + x e_2}, \quad 0 \leq x < \infty. \quad (3.178)$$

3.7.2 Stieltjes function expanded at a number of real points and infinity

(b) The case $\xi < \mathbf{x}_N = \min(\mathbf{x}_j, j = 1, 2, \dots, N)$ The initial input data for estimating $f_1(x)$ is

$$f_1(x)_{\mathbf{x}}^{\mathbf{r}}, \quad \left(\begin{matrix} \mathbf{r} \\ \mathbf{x} \end{matrix} \right) = \left(\begin{matrix} p_1, p_2, \dots, p_N, p_\infty \\ x_1, x_2, \dots, x_N, \infty \end{matrix} \right). \quad (3.179)$$

The parametric input one $f_1^{\xi, \eta}(x)_{\mathbf{x}}^{\mathbf{p}}$ associated with (3.179) takes the forms

$$f_1^{\xi, \eta}(x)_{\mathbf{x}}^{\mathbf{r}}, \quad \left(\begin{matrix} \mathbf{r} \\ \mathbf{x} \end{matrix} \right) = \left(\begin{matrix} p_1, p_2, \dots, p_N, p_\infty, 1 \\ x_1, x_2, \dots, x_N, \infty, \xi \end{matrix} \right). \quad (3.180)$$

Due to (3.180), (3.88) and (3.79) we obtain

$$F_{P+p_\infty, 1}^{x_N, \infty}(x, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k - \delta_{kN}} \frac{g_j}{1 + (x - x_k)e_{j+1} + (x - x_k)} \times \frac{F_{2, P-1}^{x_N, \infty}(x, u, e_P)}{1},$$

$$F_{2, P-1}^{x_N, \infty}(x, u) = g_{P-1} F_2(x - x_N, u, e_P), \quad (3.181)$$

$$F_2(x, u, e_P) = \frac{-u}{1 - x e_P u} \quad \text{if} \quad -1 \leq u \leq 0.$$

The multipoint Padé approximants $F_{P+p_\infty, 1}^{x_N, \infty}(x, 0)$ and $F_{P+p_\infty, 1}^{x_N, \infty}(x, -1)$ satisfy the inequalities (cf. Theorem 3.21)

$$\begin{aligned} (-1)^{L_{P+p_\infty}(x)} (F_{P+p_\infty, 1}^{x_N, \infty}(x, 0) &\leq (-1)^{L_{P+p_\infty}(x)} f_1(x) \\ &\leq (-1)^{L_{P+p_\infty}(x)} F_{P+p_\infty, 1}^{x_N, \infty}(x, -1), \end{aligned} \quad (3.182)$$

where

$$L_{P+p_\infty}(x) = \sum_{j=1}^N p_j H(x - x_j) + 1, \quad j = 1, 2, \dots, N, \quad 0 \leq x < \infty. \quad (3.183)$$

(c) The case $\xi < \mathbf{x}_1 = \min(\mathbf{x}_j, j = 2, 3, \dots, N)$ Consider again the initial input data (3.179). The parametric power expansions $f_1^{\xi, \eta}(x)_{\mathbf{x}}^{\mathbf{p}}$ associated with (3.179) are given by (cf. (3.180)) From (3.89) we obtain

$$F_{P+p_\infty, 1}^{x_1, \infty}(x, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (x - x_k)e_{j+1} + (x - x_k)} \times \frac{F_{1, P}^{x_1, \infty}(x, u, e_P)}{1},$$

$$F_{1, P}^{x_1, \infty}(x, u, e_P) = W_P^{x_1, \infty}(e_P) F_1(x - x_1, u), \quad (3.184)$$

$$F_1(x, u) = (1 + u), \quad -1 \leq u \leq 0.$$

The multipoint Padé approximants $F_{P+p_\infty, 1}^{x_1, \infty}(x, 0)$ and $F_{P+p_\infty, 1}^{x_1, \infty}(x, -1)$ satisfy the inequalities (cf. (3.184))

$$\begin{aligned} (-1)^{L_{P+p_\infty}(x)} F_{P+p_\infty, 1}^{x_1, \infty}(x, 0) &\leq (-1)^{L_{P+p_\infty}(x)} f_1(x) \\ &\leq (-1)^{L_{P+p_\infty}(x)} F_{P+p_\infty, 1}^{x_1, \infty}(x, -1). \end{aligned} \quad (3.185)$$

(d) *The cases $\xi < \mathbf{x}_N = \min(\mathbf{x}_j, j = 1, 2, \dots, N - 1)$ and $\xi < \mathbf{x}_1 = \min(\mathbf{x}_j, j = 2, 3, \dots, N)$* Let us turn our attention to the bounding functions $F_{P+p_\infty,1}^{x_1,\infty}(x, u)$ and $F_{P+p_\infty,1}^{x_N,\infty}(x, u)$ given by

$$F_{P+p_\infty,1}^{x_1,\infty}(x, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j^{x_1}}{1 + (x - x_k)e_{j+1}^{x_1} + (x - x_k)} \times \frac{F_{1,P}^{x_1,\infty}(x, u, e_P)}{1}, \tag{3.186}$$

$$F_{P+p_\infty,1}^{x_N,\infty}(x, u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k - \delta_{kN}} \frac{g_j^{x_N}}{1 + (x - x_k)e_{j+1}^{x_N} + (x - x_k)} \times \frac{F_{2,P-1}^{x_N,\infty}(x, u, e_P)}{1},$$

generated by (3.179), cf. (3.184) and (3.181). From the Theorem 3.20, it follows that even though the coefficients $g_j^{x_1}, e_{j+1}^{x_1}$ and $g_j^{x_N}, e_{j+1}^{x_N}$ are different the functions (3.186₁) and (3.186₂) do coincide

$$F_{P+p_\infty,1}^{x_1,\infty}(x, 0) = F_{P+p_\infty,1}^{x_N,\infty}(x, 0), \quad F_{P+p_\infty,1}^{x_1,\infty}(x, -1) = F_{P+p_\infty,1}^{x_N,\infty}(x, -1). \tag{3.187}$$

As an example illustrating the identities (3.91) we consider the truncated power expansions of $f_1(x)$

$$f_1(x)_{x_1}^1 = 1 + O(x - x_1), \quad f_1(x)_{x_2}^1 = \frac{1}{7} + O(x - x_2), \quad f_1(x)_{x_3}^1 = 1 + O\left(\frac{1}{x}\right), \tag{3.188}$$

$$x_1 = 0, \quad x_2 = 3, \quad x_3 = \infty$$

and

$$f_1(x)_{x_1}^1 = \frac{1}{7} + O(x - x_1), \quad f_1(x)_{x_2}^1 = 1 + O(x - x_2), \quad f_1(x)_{x_3}^1 = 1 + O\left(\frac{1}{x}\right), \tag{3.189}$$

$$x_1 = 3, \quad x_2 = 0, \quad x_3 = \infty.$$

For the cases (3.188) and (3.189) the relations (3.186₁) and (3.186₂) yield

$$F_{3+1,1}^{x_1,\infty}(x, u) = \frac{1}{1 + x + \frac{x}{1 + (x - 3)F_{1,3}^{x_1,\infty}(x, u, 0)}}, \quad F_{1,3}^{x_1,\infty}(x, u, 0) = \frac{1}{3}(1 + u), \tag{3.190}$$

$$F_{3+1,1}^{x_2,\infty}(x, u) = \frac{\frac{1}{7}}{1 + \frac{1}{7}(x - 3) + (x - 3)F_{2,2}^{x_2,\infty}(x, u, 0)}, \quad F_{2,2}^{x_2,\infty}(x, u, 0) = -\frac{1}{7}u.$$

It can be easily checked that

$$F_{3+1,1}^{x_1,\infty}(x, 0) = F_{3+1,1}^{x_2,\infty}(x, 0), \quad F_{3+1,1}^{x_1,\infty}(x, -1) = F_{3+1,1}^{x_2,\infty}(x, -1). \tag{3.191}$$

In spite of the seemingly different structures of the T -continued fraction expansions of $f_1(x)$ (3.190) the T -bounding functions $F_{2+1,1}^{x_1,\infty}(x, u)$ and $F_{2+1,1}^{x_2,\infty}(x, u)$ coincide (cf. (3.191)).

3.7.3 Series of Stieltjes with a leading coefficient $f_1(\xi) = \eta$

(e) *The case $\xi < \min(\mathbf{x}_j, j = 2, 3, \dots, N)$ and $\mathbf{f}_1(\xi) = \eta$* Consider the truncated power series $f_1(x)_x^p$ with the coefficient $f_1(\xi)$ equal to η

$$f_1^{\xi,\eta}(x)_x^p, \quad \left(\begin{matrix} \mathbf{r} \\ \mathbf{x} \end{matrix}\right) = \left(\begin{matrix} p_1, p_2, \dots, p_N, p_\infty, 1 \\ x_1, x_2, \dots, x_N, \infty, \xi \end{matrix}\right), \quad f_1^{\xi,\eta}(\xi) = \eta. \tag{3.192}$$

From (3.192), it follows the P – th order bounding function

$$F_{P+p_\infty,1}^{\xi,\eta}(x,u) = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (x-x_k)e_{j+1} + (x-x_k)} \times \frac{F_{1,P}^{\xi,\eta}(x,u,e_P)}{1}, \quad (3.193)$$

$$F_{1,P}^{\xi,\eta}(x,u,e_P) = W_P^{\xi,\eta}(e_P)F_1(x-\xi,u), \quad F_1(x,u) = 1+u, \quad -1 \leq u \leq 0.$$

By substituting

$$u = 0, \quad x = \xi, \quad F_{P+p_\infty,1}^{\xi,\eta}(\xi,0) = \eta, \quad F_1(x-\xi,0) = 1 \quad (3.194)$$

into (3.193) we obtain the equality

$$\eta = \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (\xi-x_k)e_{j+1} + (\xi-x_k)} \times \frac{W_P^{\xi,\eta}(e_P)}{1} \quad (3.195)$$

determining $W_P^{\xi,\eta}(e_P)$. From (3.64)-(3.65) we have

$$f_1(x) \in \Phi_{P+p_\infty,1}^{\xi,\eta}(x). \quad (3.196)$$

In order to illustrate the case (3.193) we consider the truncated power expansions

$$f_1(x)_2^1 = 0.18073 + O(x-2), \quad f_1(x)_\infty^1 = \frac{1}{x} \left(1 + O\left(\frac{1}{x}\right) \right), \quad (3.197)$$

$$f_1(x)_{-1}^{+1} = \eta + O(x-\xi), \quad \xi = -1, \quad \eta = 0.4694$$

of the Stieltjes function

$$f_1(x) = \frac{1}{x} \left(1 + \frac{2.5}{x} \ln \frac{1+0.1x}{1+0.5x} \right). \quad (3.198)$$

First order bounds The functions $L_1(x)$, $F_{1,1}(x,u)$, $F_{1,1}(x,0)$, $F_{1,1}(x,-1)$ computed from $f_1(x)_{-1}^{+1}$ take the forms (cf. (3.183) and (3.193))

$$\begin{aligned} L_1(x) &= H(x+1), \quad F_{1,1}(x,u) = 0.4694(1+u), \\ (-1)^{H(x+1)} 0.4694 &\leq (-1)^{H(x+1)} f_1(x) \leq 0. \end{aligned} \quad (3.199)$$

From (3.199) we have

$$0 \leq f_1(x) \leq 0.46940 \quad \text{for} \quad -1 \leq x < \infty. \quad (3.200)$$

Second order bounds From the expansions $f_1(x)_2^1$ and $f_1(x)_{-1}^{+1}$, it follows $L_2(x)$, $F_{2,1}(x,u)$, $F_{2,1}(x,0)$ and $F_{2,1}(x,-1)$

$$\begin{aligned} L_2(x) &= H(x+1) + H(x-2), \quad F_{2,1}(x,u) = \frac{0.18073}{1 + 0.2050(x-2)(1+u)}, \\ (-1)^{H(x+1)+H(x-2)} \frac{0.18073}{1 + 0.2050(x-2)} &\leq (-1)^{H(x+1)+H(x-2)} f_1(x), \end{aligned} \quad (3.201)$$

$$(-1)^{H(x+1)+H(x-2)} f_1(x) \leq (-1)^{H(x+1)+H(x-2)} 0.18073.$$

From (3.201), it follows

$$\begin{aligned} 0.18073 \leq f_1(x) &\leq \frac{0.18073}{1 + 0.2050(x - 2)} \quad \text{for } -1 \leq x \leq 2, \\ \frac{0.18073}{1 + 0.2050(x - 2)} &\leq f_1(x) \leq 0.18073 \quad \text{for } 2 \leq x < \infty. \end{aligned} \quad (3.202)$$

Third order bounds The functions $L_{2+1}(x)$, $F_{2+1,1}(x, u)$, $F_{2+1,1}(x, 0)$ and $F_{2+1,1}(x, -1)$ generated by $f_1(x)_2^1$, $f_1(x)_\infty^1$ and $f(x)_{-1}^{+1}$ are equal to

$$\begin{aligned} L_{2+1}(x) &= H(x + 1) + H(x - 2), \\ F_{2+1,1}(x, u, 1) &= \frac{0.18073}{1 + (x - 2)(0.18073 + 0.0243(1 + u))}, \end{aligned} \quad (3.203)$$

where

$$\begin{aligned} (-1)^{L_{2+1}(x)} \frac{0.18073}{1 + 0.2050(x - 2)} &\leq (-1)^{L_{2+1}(x)} f_1(x) \leq \\ &(-1)^{L_{2+1}(x)} \frac{0.18073}{1 + 0.18073(x - 2)}. \end{aligned} \quad (3.204)$$

On account of (3.201) one obtains

$$\begin{aligned} \frac{0.18073}{1 + 0.18073(x - 2)} &\leq f_1(x) \leq \frac{0.18073}{1 + 0.2050(x - 2)} \quad \text{for } -1 \leq x \leq 2, \\ \frac{0.18073}{1 + 0.2050(x - 2)} &\leq f_1(x) \leq \frac{0.18073}{1 + 0.18073(x - 2)} \quad \text{for } 2 \leq x < \infty. \end{aligned} \quad (3.205)$$

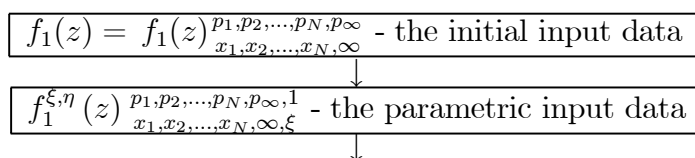
The fundamental T -inequalities (3.192)-(3.205) are new. They generalize the S -ones (2.172) derived in Chapter 2, see also [15, 60, 71] and [27, 28]).

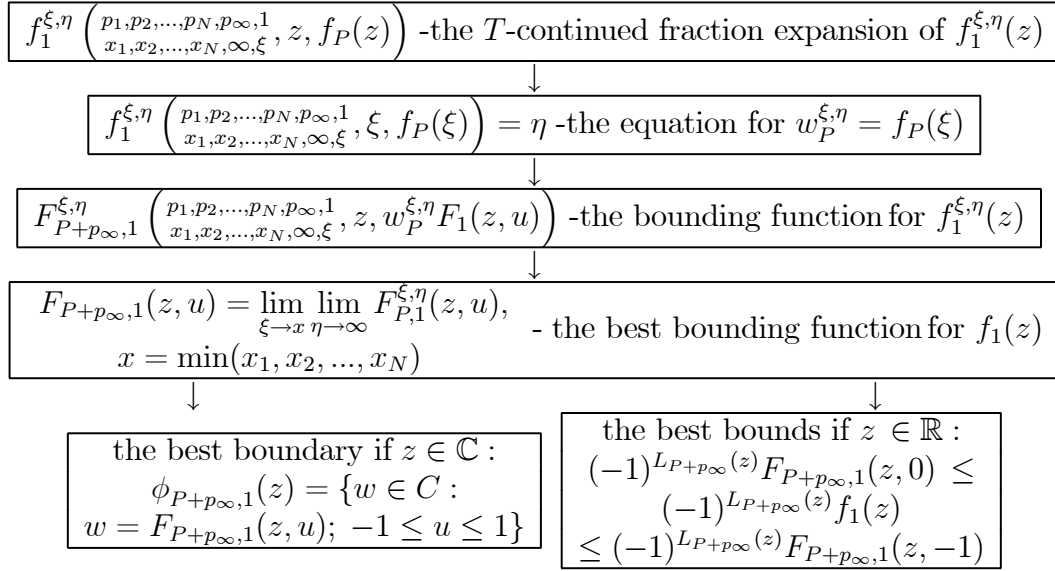
3.8 Summary and final remarks about TMC FM

In this chapter we established the new T - Multipoint Continued Fraction Method of an estimation a Stieltjes function $f_1(z)$. We prove that the T -estimates of $f_1(z)$ obtained via TMC FM are the best with respect to the power expansions of $f_1(z)$ available at real points and infinity, cf. Theorems 3.14 and 4.2. This important result is new.

The auxiliary parameters ξ , η (2.2), the recurrence T -algorithm (3.32)- (3.34), the fundamental T - inclusion relations (3.65)-(3.66), the general T - inequalities (3.170) are the main mathematical tools of TMC FM.

The T -algorithm (3.32)- (3.34) transforms the truncated power series (3.33) first to the T -continued fraction (3.35) then to the T -bounding function (3.60) and finally to the T -estimates of $f_1(z)$ represented in the complex domain by the inclusion regions (3.61), while in the real one by the upper and lower bounds (3.170). The computational TMC FM block diagram consists of:





Note that if in the above block diagram we replace z by s and $f_1(z)$ by $\varphi_1(s)$ we obtain the TCMCFM procedure estimating the Stieltjes function $\varphi_1(s) = z f_1(z)$, see Remark 3.2.

The TCMCFM established here is the first method of the theory of an approximation of Stieltjes functions $f_1(z)$ that can incorporate into the complex and real T -estimates of $f_1(z)$ the power expansions of $f_1(z)$ at infinity.

In the next chapter we adapt the TCMCFM for computing T -bounds on the effective transport coefficients of two phase-media better then previous ones reported in literature, cf. [44].

Chapter 4

THE OPTIMUM T-ESTIMATES OF EFFECTIVE TRANSPORT COEFFICIENTS OF TWO-PHASE MEDIA

The main theoretical results of the previous chapter, i.e. the fundamental inclusion relations (3.65)-(3.66) and the general inequalities (3.170) are adapted for establishing T -multipoint continued fraction bounds on effective transport coefficients $\lambda(z) - 1$, $\lambda(z) = \lambda_e(z)/\lambda_1$, $z = \lambda_2/\lambda_1 - 1$ of two-phase media.

The T -estimates of $\lambda(z) - 1$ are optimal over the given number of coefficients of the power expansions of $(\lambda(z) - 1)/z$ constructed at finite real points and infinity. The T -bounds derived here are new and better than previous ones reported in literature, cf. [44].

4.1 Fundamental T-inclusion relations for the effective transport coefficients

To get T -bounds on macroscopic coefficients $\lambda(z) - 1$ a few modifications of the TCMCFM established in Chapter 3 should be done. Let us consider the homogenized equations determining the effective transport coefficients of two phase media (cf. (1.30)-(1.31))

$$f_1(z) = \frac{1}{|Y|} \int_Y \Theta_2(y) \frac{\partial T(y)}{\partial y_1} dy, \quad (4.1)$$

$$\frac{\partial}{\partial y_j} (1 + z\Theta_2(y)) \frac{\partial T(y)}{\partial y_j} = 0, \quad (y_i - T^{(i)}) \text{ } Y\text{-periodic,}$$

where

$$f_1(z) = \frac{\lambda(z) - 1}{z}, \quad \lambda(z) = \frac{\lambda_e(z)}{\lambda_1}, \quad z = h - 1, \quad h = \frac{\lambda_2}{\lambda_1}. \quad (4.2)$$

Here $\Theta_2(y)$, λ , λ_1 and λ_2 denote in turn: the characteristic function of inclusions, the effective coefficient of a composite, the physical constant of a matrix and the material coefficient of inclusions. Without loss of generality we assume that

$$\lambda_1 = 1. \quad (4.3)$$

The effective property $(\lambda(z) - 1)/z$ (4.1)-(4.3) has a Stieltjes integral representation (1.51) satisfying the physical restriction $(\lambda(-1) - 1)/z < 1$ (cf. [11], [29] and [44])

$$f_1(z) = \frac{\lambda(z) - 1}{z} = \int_0^1 \frac{d\gamma_1(u)}{1 + zu}, \quad d\gamma_1(u) \geq 0, \quad f_1(-1) \leq 1. \quad (4.4)$$

We limit our investigations to the case

$$\lim_{z \rightarrow +\infty} z f_1(z) = \lim_{z \rightarrow +\infty} (\lambda(z) - 1) < \infty, \quad (4.5)$$

i.e. to the inhomogeneous material consisting of a matrix with $\lambda_1 = 1$ and inclusions with $\lambda_2 \in [0, \infty]$.

Consider the power expansions of $f_1(z)$ at N real points x_j , $j = 1, 2, \dots, N$

$$f_1(z) = \frac{\lambda(z) - 1}{z} = \sum_{i=0}^{p_j-1} c_{ij}(z - x_j)^i + O((z - x_j)^{p_j}), \quad j = 1, 2, \dots, N, \quad (4.6)$$

at infinity

$$f_1(z) = \frac{\lambda(z) - 1}{z} = \frac{1}{z} \sum_{i=0}^{p_\infty-1} d_i(\infty) \left(\frac{1}{z}\right)^i + O\left(\frac{1}{z}\right)^{p_\infty} \quad (4.7)$$

and at ξ

$$f_1(z) = f_1(\xi) + O(z + 1), \quad f_1(\xi) \leq \eta, \quad (4.8)$$

where

$$\xi = -1, \quad \eta = 1. \quad (4.9)$$

Problem 4.1 *By starting from the truncated power series $\frac{\lambda(z)-1}{z}$ given by (4.6)-(4.8) we compute the optimum estimates of effective transport coefficients $\lambda(z) - 1$ of two-phase media.*

To this end we rewrite the input data (4.6)-(4.9) as follows

$$f_1^{\xi, \eta}(z) = f_1^{-1,1}(z) = f_1^{-1,1}(z)_{\mathbf{p}}, \quad (\mathbf{p}) = \begin{pmatrix} p_1, p_2, \dots, p_N, p_\infty, 1 \\ x_1, x_2, \dots, x_N, \infty, -1 \end{pmatrix}. \quad (4.10)$$

The values of the Stieltjes functions $f_1^{-1,1}(z)$ belong to the inclusion regions $\Phi_{P+p_\infty,1}^{-1,1}(z)$ (4.10)

$$f_1^{-1,1}(z) \in \Phi_{P+p_\infty,1}^{-1,1}(z). \quad (4.11)$$

From (4.11), it follows immediately

$$zf_1^{-1,1}(z) \in z\Phi_{P+p_\infty,1}^{-1,1}(z), \quad (4.12)$$

where we introduce

$$z\Phi_{P+p_\infty,1}^{-1,1}(z) = \{w \in \mathbb{C} : w = zz; z \in \Phi_{P+p_\infty,1}^{-1,1}(z)\}. \quad (4.13)$$

Thus the bounding function $zF_{P+p_\infty,1}^{-1,1}(z, u)$ estimating $zf_1^{-1,1}(z)$ is equal to (cf. (3.59)-(3.62))

$$zF_{P+p_\infty,1}^{-1,1}(z, u) = z \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{F_{1,P}^{-1,1}(z, u, e_P)}{1}. \quad (4.14)$$

Now we establish the fundamental inclusion relations for T -inclusion regions estimating $zf_1^{-1,1}(z)$ in a complex domain.

Theorem 4.2 *The T -inclusion regions $z\Phi_{P(1)+p_\infty(1),1}^{-1,1}(z)$ and $z\Phi_{P(2)+p_\infty(2),1}^{-1,1}(z)$ constructed from the non-decreasing power series of Stieltjes (see Definition 2.4)*

$$f_1^{-1,1}(z)_{\mathbf{p}(1)}, \quad (\mathbf{p}) = \begin{pmatrix} p_1(1), p_2(1), \dots, p_N(1), p_\infty(1), 1 \\ x_1, x_2, \dots, x_N, \infty, -1 \end{pmatrix} \quad (4.15)$$

and

$$f_1^{-1,1}(z)_{\mathbf{p}(2)}, \quad (\mathbf{p}) = \begin{pmatrix} p_1(2), p_2(2), \dots, p_N(2), p_\infty(2), 1 \\ x_1, x_2, \dots, x_N, \infty, -1 \end{pmatrix} \quad (4.16)$$

satisfy the relations

$$zf_1^{-1,1}(z) \in z\Phi_{P(2)+p_\infty(2),1}^{-1,1}(z) \subset z\Phi_{P(1)+p_\infty(1),1}^{-1,1}(z), \quad z \in \mathbb{C} \setminus [-\infty, -1] \quad (4.17)$$

$$P(1) = \sum_{i=1}^N p_i(1) + 1, \quad P(2) = \sum_{i=1}^N p_i(2) + 1,$$

provided that

$$P(1) \leq P(2), \quad p_\infty(1) \leq p_\infty(2). \quad (4.18)$$

Proof. By substituting in (3.65) $\xi_1 = \xi_2 = -1$, $\eta_1 = \eta_2 = 1$ and multiplying both sides of (3.65) by z we obtain the fundamental inclusion relations (4.17)-(4.18). ■

The general T -inclusion relations (4.17)-(4.18) have a consequence that T -inclusion regions $z\Phi_{P+p_\infty,1}^{-1,1}(z)$ form the optimal estimates of the effective transport coefficients $\lambda(z) - 1$ obtainable from the given number of coefficients ($P + p_\infty$) and that the use of additional coefficients (higher $P + p_\infty$) does not worsen $z\Phi_{P+p_\infty,1}^{-1,1}(z)$. Thus the T -inclusion relations (4.17)-(4.18) are fundamental for an estimating of the effective transport coefficients $\lambda(z) - 1$ from the input data given by (4.6)-(4.9).

4.1.1 Particular T -estimates of effective transport coefficients of two-phase media in a complex domain

Let us focus our attention on the general T -bounding functions $zF_{P+p_\infty,1}^{-1,1}(z, u)$ (4.14) estimating the effective transport coefficients $\lambda(z) - 1$

$$zF_{P+p_\infty,1}(z, u) = z \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)e_{j+1} + (z - x_k)} \times \frac{F_{1,P}(z, u, e_P)}{1}. \quad (4.19)$$

Here for the sake of simplicity the indices $-1, 1$ are omitted. Now we compare the T -estimates of $(\lambda(z) - 1)$ given by (4.19) with the earlier bounds on $(\lambda(z) - 1)$ reported in literature [14, 42, 44, 53, 67].

a) The case $\mathbf{p}_1 > 0$, $\mathbf{p}_2 > 0$, $\mathbf{p}_3 > 0$, ..., $\mathbf{p}_N > 0$, $\mathbf{p}_\infty = 0$. The T -bounding function (4.19) reduces to the S -bounding one (2.48) derived in Chapter 2

$$zF_{P,1}(z, u) = z \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (z - x_k)} \times \frac{F_{1,P}(z, u, 0)}{1}. \quad (4.20)$$

The S -estimates (4.20) of the effective transport coefficients $\lambda(z) - 1$ are new.

b) The case $\mathbf{p}_1 > 0$, $\mathbf{p}_2 = 1$, $\mathbf{p}_3 = 1$, ..., $\mathbf{p}_N = 1$, $\mathbf{p}_\infty = 0$. From (4.20) we obtain at once

$$zF_{P,1}(z, u) = z \prod_{j=P_0+1}^{P_1} \frac{g_j}{1 + z} \times z \prod_{k=2}^N \prod_{j=P_1+k}^{P_1+k} \frac{g_k}{1 + (z - x_k)} \times \frac{F_{1,P}(z, u, 0)}{1}. \quad (4.21)$$

The estimates $zF_{P,1}(z, u)$ of $\lambda(z) - 1$ derived by us (see 4.21), by Milton [42] and by Bergman [14] lead to the same inclusion regions $z\Phi_{P,1}(z)$ estimating $\lambda(z) - 1$.

c) The case $\mathbf{p}_1 > 0$, $\mathbf{p}_2 = 0$, $\mathbf{p}_3 = 0$, ..., $\mathbf{p}_N = 0$, $\mathbf{p}_\infty = 0$. We obtain further simplifications of (4.21)

$$zF_{P,1}(z, u) = z \prod_{j=P_0+1}^{P_1} \frac{g_j}{1 + z} \times \frac{F_{1,P}(z, u, 0)}{1}. \quad (4.22)$$

The formula (4.22) was derived by Tokarzewski and Telega [67] and applied to compute the effective dielectric constants of regular arrays of spheres.

d) The case $\mathbf{p}_1 = \mathbf{1}, \mathbf{2}, \mathbf{p}_2 = \mathbf{0}, \mathbf{p}_3 = \mathbf{0}, \dots, \mathbf{p}_N = \mathbf{0}, \mathbf{p}_\infty = \mathbf{0}$. The formula (4.19) leads to the bounding functions

$$zF_{P,1}(z, u) = z \bigvee_{j=1}^1 \frac{g_j}{1+z} \times \frac{F_{1,P}(z, u, 0)}{1} \quad (4.23)$$

and

$$zF_{P,1}(z, u) = z \bigvee_{j=1}^2 \frac{g_j}{1+z} \times \frac{F_{1,P}(z, u, 0)}{1}, \quad (4.24)$$

which are the complex counterparts of the Wiener [73] and Hashin-Shtrikman [30] bounds on $\lambda(z) - 1$ defined in the real domain.

4.1.2 Illustrative example of an evaluation of the complex T-estimates

As an example of a practical evaluations of the T -inclusion regions estimating $\lambda(z) - 1$ (see Theorem 4.2) we consider a dielectric consisting of equally-sized cylinders embedded in an infinite matrix, cf. Fig. 4.1. To this end we set: $\varepsilon_1, \varepsilon_2$ - dielectric constants of a matrix and inclusions, $z = ((\varepsilon_2/\varepsilon_1) - 1)$ - nondimensional constant of cylinders, $\varepsilon(z) = \varepsilon_e(z)/\varepsilon_1$ - effective coefficient of a composite, ρ - radius of cylinders, $\varphi = \pi\rho^2$ - volume fraction of inclusions. For isotropic symmetry the system of equations determining the effective

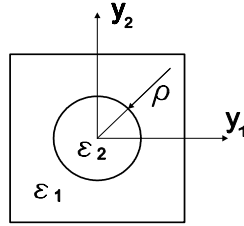


Fig. 4.1 Unit cell for square array of cylinders: $\varepsilon_1, \varepsilon_2$ — dielectric constants of a matrix and inclusion, respectively.

constant $(\varepsilon(z) - 1)/z$ reduces to (cf. (1.30)-(1.31))

$$\frac{\varepsilon(z) - 1}{z} = \frac{1}{|Y|} \int_Y \Theta_2(y) \frac{\partial T(y)}{\partial y_1} dy, \quad (4.25)$$

$$\frac{\partial}{\partial y_i} \frac{\partial T(y)}{\partial y_i} = -z \frac{\partial}{\partial y_i} \left(\Theta_2(y) \frac{\partial T(y)}{\partial y_i} \right), \quad (y_1 - T) \text{ } Y\text{-periodic.} \quad (4.26)$$

Here $\Theta_2(y)$ is the characteristic function of cylinders. The asymptotic solutions of the equations (4.25) and (4.26) is reported in Section 1.2 of Chapter 1

$$\frac{\varepsilon(z) - 1}{z} = \langle y_1, T \rangle = \langle y_1, (1 + z\Gamma)^{-1} y_1 \rangle = \langle y_1, y_1 \rangle + \langle y_1, \Gamma y_1 \rangle z + O(z^2), \quad (4.27)$$

where

$$T = (1 + z\Gamma)^{-1} y_1 = \sum_{k=0}^{\infty} (\Gamma^k y_1) z^k. \quad (4.28)$$

For macroscopically isotropic composite materials the first two coefficients $\langle y_1, y_1 \rangle$ and $\langle y_1, \Gamma y_1 \rangle$ of the power expansion of $\frac{\varepsilon(z) - 1}{z}$ (4.27) are evaluated in [11]

$$\langle y_1, y_1 \rangle = \varphi, \quad \langle y_1, \Gamma y_1 \rangle = \frac{1}{2} \varphi (1 - \varphi). \quad (4.29)$$

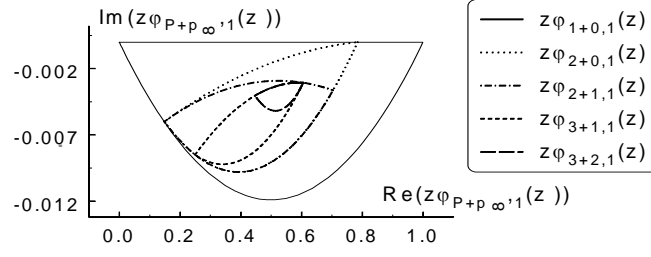


Fig. 4.2 The complex boundaries $z\phi_{P+p\infty,1}(z)$ estimating the effective dielectric constant $\lambda(z) - 1$ of a square array of cylinders, cf. (4.36), $\varphi = 0.785$, $z = 20 + i$.

Hence we have

$$\frac{\varepsilon(z) - 1}{z} = c_0(0) + c_1(0)z + O(z^2), \quad (4.30)$$

where (cf. (4.29))

$$c_0(0) = \varphi = \pi\rho^2, \quad c_1(0) = b = -\frac{1}{2}\varphi(1 - \varphi). \quad (4.31)$$

The power expansion of $(\varepsilon(z) - 1)/z$ at $z = \infty$ is evaluated by McPhedran *et al.* [39]

$$\frac{\varepsilon(z) - 1}{z} = \frac{1}{z} \left(d_0(\infty) + d_1(\infty)\frac{1}{z} + O\left(\frac{1}{z}\right)^2 \right), \quad (4.32)$$

$$d_0(\infty) = A = [\pi(w - 1) - 1], \quad d_1(\infty) = B = -2\pi w(w - 1) \ln w, \quad w = \sqrt{\frac{\pi}{\pi - 4\varphi}}. \quad (4.33)$$

From (4.8), it follows

$$f_1(z) = f_1(-1) + O(z + 1), \quad f_1(-1) \leq 1, \quad f_1(z) = \frac{\varepsilon(z) - 1}{z}. \quad (4.34)$$

By starting from (4.30)-(4.31), (4.32)-(4.33) and (4.34) the sequences of the T -bounding functions

$$zF_{1,1}(z, u), \quad zF_{2,1}(z, u), \quad zF_{2+1,1}(z, u), \quad zF_{3+1,1}(z, u), \quad zF_{3+2,1}(z, u) \quad (4.35)$$

and the complex T -boundaries

$$z\phi_{1,1}(z), \quad z\phi_{2,1}(z), \quad z\phi_{2+1,1}(z), \quad z\phi_{3+1,1}(z), \quad z\phi_{3+2,1}(z) \quad (4.36)$$

are evaluated in the analytical forms. For example for $zF_{3+2,1}(z, u)$ we obtain

$$zF_{3+2,1}(z, u) = \frac{zg_1}{1 + e_2z + \frac{g_2z}{1 + e_3z + (w_3 - e_3)F_1(z + 1, u)}}, \quad (4.37)$$

$$g_1 = \varphi, \quad e_2 = \frac{\varphi}{A}, \quad g_2 = -\frac{\varphi}{A} - \frac{b}{\varphi}, \quad e_3 = \frac{\varphi + Ab}{A^2 + \varphi B} \frac{A}{\varphi}, \quad w_3 = \frac{g_1 + e_2 + g_2 - 1}{g_1 + e_2 - 1}, \quad (4.38)$$

g_1	e_2	g_2	e_3	w_3
0.785000	0.005756	0.101744	0.108299	0.513753

(4.39)

The complex boundaries (4.36) are evaluated and depicted in Fig. 4.2. For more examples of estimations of complex coefficients by TMC FM we refer the reader to Section 4.3.

4.2 Fundamental inequalities for T- bounds on the real effective transport coefficients

Now we establish the fundamental inequalities for T -multipoint Padé approximants $x F_{P+p_\infty,1}(x, j)$, $j = 0, -1$ to the transport coefficient $\lambda(x) - 1$ of a two-phase medium, where $x = (\lambda_1/\lambda_2) - 1 \in \mathbb{R}$.

Theorem 4.3 *Consider the non-decreasing power expansions of effective transport coefficients (see (2.7)- (2.9))*

$$f_1(x) = \sum_{i=0}^{p_j} c_{ij}(x - x_j)^i + O((x - x_j)^{p_j}), \quad j = 1, \dots, N,$$

$$f_1(x) = \sum_{i=0}^{p_\infty} d_{i\infty} \left(\frac{1}{x}\right)^i + O\left(\left(\frac{1}{x}\right)^{p_j}\right), \quad f_1(x) = 1 + O(x + 1), \quad (4.40)$$

$$f_1(x) = \frac{\lambda(x) - 1}{x}$$

and accompanying them the $L_{P+p_\infty}(x)$ - characteristic functions, see (2.6). The diagonal and overdiagonal T -multipoint Padé approximants $F_{P+p_\infty,1}(x, J)$, $x \in \mathbb{R} \setminus [-\infty, \xi]$, $J = 0, 1$ to the power expansions (4.40) satisfy the following inequalities

$$\begin{aligned} (-1)^{R_{P+p_\infty}-1(x)} x F_{P+p_\infty-1,1}(x, 0) &\geq (-1)^{R_{P+p_\infty}-1(x)} x F_{P+p_\infty,1}(x, 0), \\ (-1)^{R_{P+p_\infty}-1(x)} x F_{P+p_\infty-1,1}(x, -1) &\leq (-1)^{R_{P+p_\infty}-1(x)} x F_{P+p_\infty,1}(x, -1), \\ (-1)^{R_{P+p_\infty}(x)} x F_{P+p_\infty,1}(x, 0) &\geq (-1)^{R_{P+p_\infty}(x)} (\lambda(x) - 1) \geq \\ &(-1)^{R_{P+p_\infty}(x)} x F_{P+p_\infty,1}(x, -1), \end{aligned} \quad (4.41)$$

where

$$R_{P+p_\infty}(x) = L_{P+p_\infty}(x) + H(x). \quad (4.42)$$

Proof. By substituting $\xi = -1$ and $\eta = 1$ in (3.170) and multiplying both sides of the inequalities (3.170) by x we obtain:

If $-1 \leq x \leq 0$ then

$$\begin{aligned} (-1)^{L_{P-1}(x)} x F_{P+p_\infty-1,1}(x, 0) &\geq (-1)^{L_{P-1}(x)} x F_{P+p_\infty,1}(x, 0), \\ (-1)^{L_{P-1}(x)} x F_{P+p_\infty-1,1}(x, -1) &\leq (-1)^{L_{P-1}(x)} x F_{P+p_\infty,1}(x, -1), \\ (-1)^{L_P(x)} x F_{P+p_\infty,1}(x, 0) &\geq (-1)^{L_P(x)} x f_1(x) \geq (-1)^{L_P(x)} x F_{P+p_\infty,1}(x, -1). \end{aligned} \quad (4.43)$$

If $0 \leq x < \infty$ then

$$\begin{aligned} (-1)^{L_{P-1}(x)} x F_{P+p_\infty-1,1}(x, 0) &\leq (-1)^{L_{P-1}(x)} x F_{P+p_\infty,1}(x, 0), \\ (-1)^{L_{P-1}(x)} x F_{P+p_\infty-1,1}(x, -1) &\geq (-1)^{L_{P-1}(x)} x F_{P+p_\infty,1}(x, -1), \\ (-1)^{L_P(x)} x F_{P+p_\infty,1}(x, 0) &\leq (-1)^{L_P(x)} x f_1(x) \leq (-1)^{L_P(x)} x F_{P+p_\infty,1}(x, -1). \end{aligned} \quad (4.44)$$

Due to (4.42) the inequalities (4.43)-(4.44) and (4.41) coincide. ■

The T -multipoint Padé approximants $xF_{P+p_\infty,1}(x, j)$, $j = 0, -1$ form the optimal upper and lower bounds on $\lambda(x) - 1$ obtainable using only the given number of coefficients ($P + p_\infty$) and that the use of additional coefficients (higher ($P + p_\infty$)) does not worsen the bounds $xF_{P+p_\infty,1}(x, j)$, $j = 0, -1$. Thus the Theorem 4.3 is fundamental for it provides, with respect to the given terms of the truncated power series $(\lambda(x) - 1)/x$, the optimum bounds on $\lambda(x) - 1$.

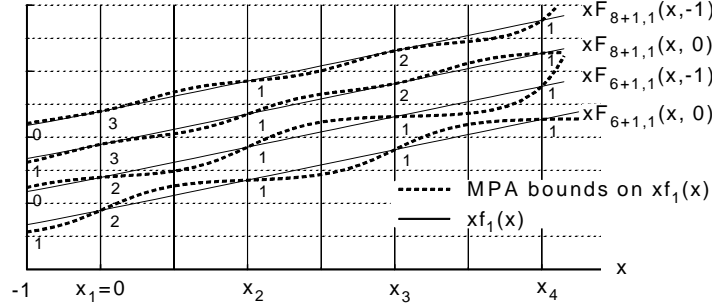


Fig. 4.3 Sketch illustrating the fundamental inequalities (4.41) for the multipoint Padé bounds $xF_{6+1,1}(x, 0)$, $xF_{6+1,1}(x, -1) + 5$ and $xF_{8+1,1}(x, 0) + 10$, $xF_{8+1,1}(x, -1) + 15$ on the effective transport coefficient $\lambda(x) - 1$. The numbers of coefficients of power expansions of $f_1(x)$ at $-1, 0, x_2, x_3, x_4$ incorporated into the bounds $xF_{P+p_\infty,1}(x, u) + C$, $u = -1, 0$ are depicted on the graph.

By way of the illustration of Theorem 4.3 the Padé approximants

$$xF_{6+1,1}(x, 0), xF_{6+1,1}(x, -1) ; xF_{8+1,1}(x, 0), xF_{8+1,1}(x, -1) \quad (4.45)$$

estimating the effective transport coefficient

$$xf_1(x) = \lambda(x) - 1 \quad (4.46)$$

are sketched qualitatively in Fig. 4.3. The numbers of the coefficients of the expansions of $xf_1(x)$ at $-1, x_1, x_2, x_4$ incorporated into the T -Padé bounds (4.45) are specified in Fig. 4.3. By summing them in a proper way we arrive at the characteristic functions $R_6(x)$ and $R_8(x)$ associated with the estimations (4.45). For example we have (cf. Fig. 4.3):

$$R_6(x) = 5, R_8(x) = 6 \text{ if } x_2 < x < x_3 \quad (4.47)$$

and

$$R_6(x) = 7, R_8(x) = 9, \text{ if } x_4 < x < \infty. \quad (4.48)$$

By substituting into (4.41) the characteristic functions (4.47) and (4.48) we obtain (cf. Fig. 4.3)

$$(-1)^5 xF_{6+1,1}(x, 0) \geq (-1)^5 (\lambda(x) - 1) \geq (-1)^5 xF_{6+1,1}(x, -1), \quad x_2 < x < x_3, \quad (4.49)$$

$$(-1)^6 xF_{8+1,1}(x, 0) \geq (-1)^6 (\lambda(x) - 1) \geq (-1)^6 xF_{8+1,1}(x, -1), \quad x_2 < x < x_3.$$

and

$$(-1)^7 xF_{6+1,1}(x, 0) \geq (-1)^7 (\lambda(x) - 1) \geq (-1)^7 xF_{6+1,1}(x, -1), \quad x_4 < x < \infty, \quad (4.50)$$

$$(-1)^9 xF_{8+1,1}(x, 0) \geq (-1)^9 (\lambda(x) - 1) \geq (-1)^9 xF_{8+1,1}(x, -1), \quad x_4 < x < \infty.$$

From (4.41), it follows that $xF_{6+1,1}(x, 0)$, $xF_{6+1,1}(x, -1)$ and $xF_{8+1,1}(x, 0)$, $xF_{8+1,1}(x, -1)$, $-1 < x < \infty$ are the optimum bounds on $\lambda(x) - 1$ over the input data given by eight ($7+1$) and nine ($8+1$) coefficients of the truncated power series, see Fig. 4.3. Here $+1$ appearing in ($7+1$) and ($8+1$) means that one coefficient of an expansion of $(\lambda(x) - 1)/z$ at infinity is incorporated into bounds (4.50).

4.2.1 Particular T-estimates of effective transport coefficients of two-phase media in a real domain

The general T -multipoint Padé bounds on the effective transport coefficients $\lambda(x) - 1$, $x \in [-1, \infty]$ of two-phase media take the forms (cf. (4.19))

$$xF_{P+p_\infty,1}(x, u) = x \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (x - x_k)e_{j+1} + (x - x_k)} \times \frac{F_{1,P}(x, u, e_P)}{1}, \quad (4.51)$$

where $u = -1, 0$. Particular cases of the T -formula (4.51) will be discussed:

a) The case $\mathbf{p}_1 > \mathbf{0}$, $\mathbf{p}_2 = \mathbf{0}$, $\mathbf{p}_3 = \mathbf{0}$, ..., $\mathbf{p}_N = \mathbf{0}$, $\mathbf{p}_\infty > \mathbf{0}$. The inequalities (4.41)-(4.42) reduce to

$$\begin{aligned} (-1)^{R_{P+p_\infty}(x)} x F_{P+p_\infty,1}(x, 0) &\geq (-1)^{R_{P+p_\infty}(x)} (\lambda(x) - 1) \geq \\ &(-1)^{R_{P+p_\infty}(x)} x F_{P+p_\infty,1}(x, -1), \quad x \in [-1, \infty], \end{aligned} \quad (4.52)$$

$$R_{P+p_\infty}(x) = 1 + (p_1 + 1)H(x) + p_\infty H(x - \infty), \quad P = p_1 + 1,$$

where (cf.(4.51))

$$xF_{P+p_\infty,1}(x, u) = x \prod_{j=1}^{p_1} \frac{g_j}{1 + x e_{j+1} + x} \times \frac{F_{1,P}(x, u, e_P)}{1}, \quad u = -1, 0. \quad (4.53)$$

The inequalities (4.52) valid for the three-point Padé bounds (4.53) were derived by Tokarzewski and Telega in [68], see also [54, 58, 59].

b) The case $\mathbf{p}_1 > \mathbf{0}$, $\mathbf{p}_2 > \mathbf{0}$, $\mathbf{p}_3 > \mathbf{0}$, ..., $\mathbf{p}_N > \mathbf{0}$, $\mathbf{p}_\infty = \mathbf{0}$. The inequalities (4.41₃)-(4.42) take the form

$$(-1)^{R_P(x)} x F_{P,1}(x, 0) \geq (-1)^{R_P(x)} (\lambda(x) - 1) \geq (-1)^{R_P(x)} x F_{P,1}(x, -1),$$

$$R_P(x) = L_P(x) + H(x) = 1 + \sum_{k=1}^N p_k H(x - x_k) + H(x), \quad (4.54)$$

$$P = 1 + \sum_{k=1}^N p_k, \quad x \in (-1, \infty),$$

while (4.51) reduces to

$$xF_{P+p_\infty,1}(x, u) = x \prod_{k=1}^N \prod_{j=P_{k-1}+1}^{P_k} \frac{g_j}{1 + (x - x_k)} \times \frac{F_{1,P}(x, u, 0)}{1}, \quad u = -1, 0. \quad (4.55)$$

The estimates (4.55) and the inequalities (4.54) coincide with the bounds derived in [71] and rigorously proved in [27], cf. also [28, 52, 60].

c) The case $\mathbf{p}_1 > \mathbf{0}$, $\mathbf{p}_2 = \mathbf{1}$, $\mathbf{p}_3 = \mathbf{1}$, ..., $\mathbf{p}_N > \mathbf{1}$, $\mathbf{p}_\infty = \mathbf{0}$. From the inequalities (4.41₃)-(4.42), it follows

$$(-1)^{R_P(x)} x F_{P,1}(x, 0) \geq (-1)^{R_P(x)} (\lambda(x) - 1) \geq (-1)^{R_P(x)} x F_{P,1}(x, -1),$$

$$R_P(x) = L_P(x) + H(x) = 1 + (p_1 + 1)H(x) + \sum_{k=2}^N H(x - x_k), \quad (4.56)$$

$$P = 1 + p_1 + N - 1, \quad x \in (-1, \infty),$$

while the relation (4.51) yields

$$xF_{P,1}(x, u) = x \prod_{j=P_0+1}^{P_1} \frac{g_j}{1+x} \times x \prod_{k=2}^N \prod_{j=P_1+k-1}^{P_1+k-1} \frac{g_k}{1+(x-x_k)} \times \frac{F_{1,P}(x, u, 0)}{1}, \quad u = -1, 0. \quad (4.57)$$

Earlier Milton [42] and independently Bergman [14] derived the estimates (4.57), but they did not establish the inequalities for them, see (4.56). On account of that the relations (4.56) are new.

d) The case $\mathbf{p}_1 > 0$, $\mathbf{p}_2 = 0$, $\mathbf{p}_3 = 0$, ..., $\mathbf{p}_N = 0$, $\mathbf{p}_\infty = 0$. Further simplifications of (4.56)-(4.57) are obtained

$$\begin{aligned} (-1)^{R_P(x)} xF_{P,1}(x, 0, 0) &\geq (-1)^{R_P(x)} (\lambda(x) - 1) \geq (-1)^{R_P(x)} xF_{P,1}(x, -1, 0), \\ R_P(x) &= L_P(x) + H(x) = 1 + (p_1 + 1)H(x), \quad P = 1 + p_1, \quad x \in (-1, \infty), \end{aligned} \quad (4.58)$$

where

$$xF_{1,P}(x, u, 0) = x \prod_{j=1}^{P_1} \frac{g_j}{1+x} \times \frac{F_{1,P}(x, u, 0)}{1}, \quad u = -1, 0. \quad (4.59)$$

The inequalities (4.58) are applied by Tokarzewski [53], Tokarzewski and Telega [67] for an investigation of the effective thermal conductivity of regular arrays of cylinders, see also [21, 22, 38].

e) The case $\mathbf{p}_1 = 1$, $\mathbf{p}_2 = 0$, $\mathbf{p}_3 = 0$, ..., $\mathbf{p}_N = 0$, $\mathbf{p}_\infty = 0$. The relations (4.41₃)-(4.42) and (4.51) yield

$$\begin{aligned} (-1)^{R_2(x)} xF_{2,1}(x, 0) &\geq (-1)^{R_2(x)} (\lambda(x) - 1) \geq (-1)^{R_2(x)} xF_{2,1}(x, -1), \\ R_2(x) &= L_2(x) + H(x) = 1 + 2H(x), \quad x \in (-1, \infty) \end{aligned} \quad (4.60)$$

and

$$xF_{2,1}(x, u) = x \prod_{j=1}^1 \frac{g_j}{1+x} \times \frac{F_{1,2}(x, u, 0)}{1}, \quad u = -1, 0. \quad (4.61)$$

The bounds $xF_{2,1}(x, 0)$ and $xF_{2,1}(x, -1)$ take the explicit form (cf. (4.61))

$$xF_{2,1}(x, 0) = \frac{\varphi x}{1 + (1 - \varphi)x}, \quad xF_{2,1}(x, -1) = \varphi x, \quad (4.62)$$

where φ denotes the volume fraction of inclusions. Hence the inequalities (4.60) reduce to

$$\begin{aligned} (-1)^{1+2H(x)} \frac{\varphi x}{1 + (1 - \varphi)x} &\geq (-1)^{1+2H(x)} (\lambda(x) - 1) \geq \\ &(-1)^{1+2H(x)} \varphi x, \quad x \in (-1, \infty). \end{aligned} \quad (4.63)$$

From (4.63), it follows immediately

$$\frac{\varphi x}{1 + (1 - \varphi)x} \leq (\lambda(x) - 1) \leq \varphi x, \quad x \in (-1, \infty). \quad (4.64)$$

The relations (4.64) coincide with the classical Wiener bounds [73].

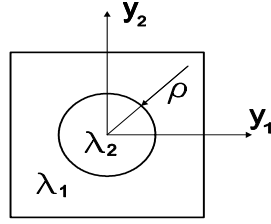


Fig. 4.4 Unit cell for square array of cylinders: λ_1 , λ_2 —thermal conductivities of a matrix and inclusion, respectively.

f) **The case** $\mathbf{p}_1 = \mathbf{2}$, $\mathbf{p}_2 = \mathbf{0}$, $\mathbf{p}_3 = \mathbf{0}$, ..., $\mathbf{p}_N = \mathbf{0}$, $\mathbf{p}_\infty = \mathbf{0}$. The relations (4.51) yield the Padé bounds

$$xF_{3,1}(x, u, 0) = x \bigvee_{j=1}^2 \frac{g_j}{1+x} \times \frac{F_{1,3}(x, u, 0)}{1}, \quad u = -1, 0 \quad (4.65)$$

fulfilling the inequalities

$$\begin{aligned} (-1)^{R_3(x)} x F_{3,1}(x, 0) &\geq (-1)^{R_3(x)} (\lambda(x) - 1) \geq (-1)^{R_3(x)} x F_{3,1}(x, -1), \\ R_3(x) = L_3(x) + H(x) &= 1 + 3H(x), \quad x \in (-1, \infty). \end{aligned} \quad (4.66)$$

The bounds $xF_{3,1}(x, 0)$ and $xF_{3,1}(x, -1)$ are equal to (cf. (4.65))

$$xF_{3,1}(x, 0, 0) = \frac{\varphi x}{1 + \frac{0.5(1-\varphi)x}{1+0.5x}}, \quad xF_{3,1}(x, -1, 0) = \frac{\varphi x}{1 + 0.5(1-\varphi)x}. \quad (4.67)$$

By substituting (4.67) into (4.66) we obtain the estimates

$$\begin{aligned} (-1)^{1+3H(x)} \frac{\varphi x}{1 + \frac{0.5(1-\varphi)x}{1+0.5x}} &\geq (-1)^{1+3H(x)} (\lambda(x) - 1) \geq \\ &(-1)^{1+3H(x)} \frac{\varphi x}{1 + 0.5(1-\varphi)x}, \quad x \in (-1, \infty) \end{aligned} \quad (4.68)$$

derived earlier by Hashin-Shtrikman [30].

4.2.2 Example for an evaluation of real T-estimates

As an example of practical application of the T -multipoint Padé bounds on $\lambda(x) - 1$ (4.41) we consider a thermal conductor consisting of equally-sized cylinders regular embedded in an infinite matrix, cf. Fig. 4.4. We set: λ_1 , λ_2 —conductivity coefficients of a matrix and cylinders, $x = ((\lambda_2/\lambda_1) - 1)$ —nondimensional modulus of the cylinders, $\lambda(x) = \lambda_e(x)/\lambda_1$ —nondimensional effective conductivity, $\varphi = \pi\rho^2$ —volume fraction of inclusions, ρ —radius of cylinders. By substituting into (4.35) $z = x \in \mathbb{R}$ we get the real T -Padé bounds

$$xF_{2,1}(x, u), \quad xF_{3,1}(x, u), \quad xF_{3+2,1}(x, u), \quad u = -1, 0 \quad (4.69)$$

estimating the effective conductivity $\lambda(x) - 1$ of a square array of cylinders, see Fig. 4.5. The T -Padé estimations $xF_{3+2,1}(x, u)$, $u = -1, 0$ are better than the Wiener $xF_{2,1}(x, u)$, $u = -1, 0$ and Hashin-Shtrikman $xF_{3,1}(x, u)$, $u = -1, 0$ ones, cf. [73] and [30]. In Subsection 4.3.4 the T -Padé bounds on $(\lambda(x) - 1)/x$ narrower than (4.69) are evaluated, see also [58].

Table 4.1 Low order coefficients, c_n, g_n ($n = 1, 2, \dots, 6$) and w_n ($n = 1, 2, \dots, 7$) for evaluation of S -continued fraction bounds $F_{p,1}(x, 0)$ and $F_{p,1}(x, 1)$ for the conductivity $\lambda_e(x)$ of regular arrays of spheres

Array of spheres		n=1	n=2	n=3	n=4	n=5	n=6	n=7
$\varphi = 0.5$ simple cubic	c_n	0.5	0.0833	0.0235	0.0019	0.0043	0.0023	
	g_n	0.5	0.1667	0.1158	0.2693	0.1170	0.3203	
	w_n	1.0	0.5000	0.6667	0.8261	0.6741	0.8263	0.6162
$\varphi = 0.6$ Body-centred	c_n	0.6	0.0800	0.0149	0.0042	0.0016	0.0008	
	g_n	0.6	0.1333	0.0530	0.3376	0.0710	0.3856	
	w_n	1.0	0.4000	0.6667	0.9204	0.6331	0.8878	0.5657
$\varphi = 0.7$ Face-centred	c_n	0.7	0.0700	0.0144	0.0056	0.0028	0.0016	
	g_n	0.7	0.1000	0.1064	0.3458	0.1046	0.3381	
	w_n	1.0	0.3000	0.6667	0.8403	0.5884	0.8221	0.5872

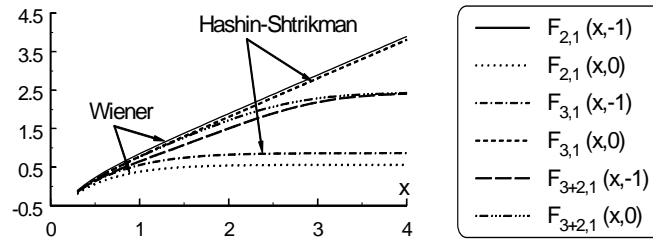


Fig. 4.5 The comparison of the mutipoint Padé bounds $xF_{2,1}(x, u)$, $xF_{3,1}(x, u)$, $xF_{3+2,1}(x, u)$, $u = -1, 0$ on effective transport coefficient $\lambda(x) - 1$ with the classical Wiener and Hashin-Shtrikman estimates. Padé bounds $xF_{3+2,1}(x, u)$, $u = -1, 0$ are narrower then Wiener and Hashin-Shtrikman ones.

4.3 Numerical examples of evaluation of effective transport coefficients by TCMFM

In this section we present a few nontrivial applications of TCMFM in the mechanics of inhomogeneous media.

4.3.1 Complex dielectric constants of spheres forming regular arrays [67]

Let us consider simple, body-centered and face-centered, cubic lattices of spheres embedded in an infinite matrix material. By $\varepsilon_e, \varepsilon_2, \varepsilon_1$ we denote the dielectric constants of a composite, spheres and matrix, respectively. For a macroscopically isotropic, two-component materials the first two coefficients of the power series developed at zero are as

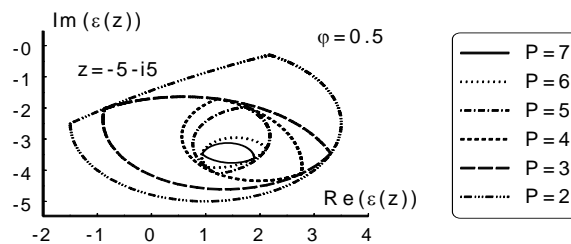


Fig. 4.6 The sequence of the lens-shaped bounds $1 + z\phi_{p,1}(z)$ on the effective dielectric constant $\varepsilon_e/\varepsilon_1$ for the simple cubic lattice of spheres.

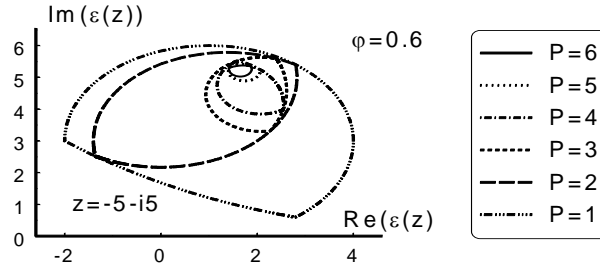


Fig. 4.7 The sequence of the lens-shaped bounds $1 + z\phi_{P,1}(z)$ on the effective dielectric constant $\varepsilon_e/\varepsilon_1$ for a body-centred cubic lattice of spheres.

follows ((4.30)-(4.31))

$$f_1(z) = \frac{\varepsilon_e(z) - \varepsilon_1}{z\varepsilon_1} = \varphi - \frac{1}{3}\varphi(1-\varphi)z + O(z^2), \quad z = \varepsilon_2/\varepsilon_1 - 1. \quad (4.70)$$

Here φ , $(1-\varphi)$ denote the volume fractions of inclusions and of a matrix, respectively. At $\xi = -1$ we can write (cf. 4.8)

$$f_1(z) \leq 1 + O(z+1). \quad (4.71)$$

Since $e_j = 0$ the T -continued fraction expansion of $f_1(z)$ reduces to the S -continued fraction one (cf. (4.70)-(4.71))

$$f_1(z) = \frac{\varphi}{1+z} \times \frac{\frac{1}{3}(1-\varphi)}{1+z} \times \frac{f_3(z)}{1}. \quad (4.72)$$

The low order S -bounding functions $zF_{P,1}(z, u)$, $p = 1, 2, 3$ take the forms (cf. (4.19) and (4.72))

$$zF_{1,1}(z, u) = zF_1(z+1, u), \quad zF_{2,1}(z, u) = \frac{\varphi z}{1+z} \times \frac{w_2 F_1(z+1, u)}{1}, \quad (4.73)$$

$$zF_{3,1}(z, u) = \frac{\varphi z}{1+z} \times \frac{\frac{1}{3}(1-\varphi)z}{1+z} \times \frac{w_3 F_1(z+1, u)}{1}. \quad (4.74)$$

Here $F_1(z, u)$ is the elementary bounding function estimating $f_1(z)$ (1.154), while the constants w_P ($P = 1, 2, 3$) are equal to

$$w_1 = 1, \quad w_2 = \varphi, \quad w_3 = \frac{2}{3}. \quad (4.75)$$

By substituting (4.75) into (4.73) and (4.74), we obtain $zF_{P,1}(z, u)$ estimating $\varepsilon_e/\varepsilon_1 - 1$ for the cases:

1) $P = 1$ — first coefficient of the series (4.71) is known:

$$zF_{1,1}(z, u) = \begin{cases} \frac{(1+u)z}{1}, & -1 \leq u \leq 0, \\ \frac{1-u}{1+zu} \frac{z}{1}, & 0 \leq u \leq 1. \end{cases} \quad (4.76)$$

Table 4.2 c_n - the coefficients of the power expansion of $\varepsilon_e/\varepsilon_1$; g_n and w_n - the coefficients of the S-continued fraction to $\varepsilon_e/\varepsilon_1$

Arrays of cylinders		n=1	n=2	n=3	n=4	n=5	n=6
$\varphi=0.75$	c_n	0.75	0.094	0.030	0.015	0.009	0.006
Square array	g_n	0.75	0.125	0.196	0.304	0.144	0.356
	w_n	1.00	0.250	0.500	0.607	0.500	0.712
$\varphi=0.88$	c_n	0.88	0.053	0.011	0.005	0.003	0.002
Hexag. array	g_n	0.88	0.060	0.146	0.354	0.169	0.331
	w_n	1.00	0.120	0.500	0.710	0.500	0.661

2) $P = 2$ – first coefficients of the series (4.70) and (4.71) are known:

$$zF_{2,1}(z, u) = \begin{cases} \frac{\varphi z}{1+z} \times \frac{(1-\varphi)(1+u)}{1}, & -1 \leq u \leq 0, \\ \frac{\varphi z}{1+z} \times \frac{(1-\varphi)\frac{1-u}{1+zu}}{1}, & 0 \leq u \leq 1. \end{cases} \quad (4.77)$$

3) $P = 3$ – two and one coefficients of the expansions (4.70) and (4.71) are given:

$$zF_{3,1}(z, u) = \begin{cases} \frac{\varphi z}{1} \times \frac{(1-\varphi)z}{3} \times \frac{2}{3} \frac{(1+u)z}{1}, & -1 \leq u \leq 0, \\ \frac{\varphi z}{1} \times \frac{(1-\varphi)z}{3} \times \frac{2}{3} \frac{1-u}{1+zu} z, & 0 \leq u \leq 1. \end{cases} \quad (4.78)$$

The TCMCFM bounds (4.76)-(4.78) coincide with the low order complex bounds derived by Milton [40] and independently by Bergman [12]. The circular arcs $1+z\phi_{1,1}(z)$, $1+z\phi_{2,1}(z)$, $1+z\phi_3(z)$ estimating the effective dielectric constant $\varepsilon_e/\varepsilon_1$ are depicted in Figs 4.6 and 4.7. To get bounds more narrow than (4.76)-(4.78) we have to incorporate in a computing algorithm many terms of a power expansion of $\varepsilon_e(z)/\varepsilon_1$ at $z = 0$. For the simple, body-centered and face-centered cubic lattices of spheres McPhedran and Milton [38] evaluated several coefficients of a power expansion of $\varepsilon_e(\alpha)/\varepsilon_1$, $\alpha = z/(z+2)$, at $\alpha = 0$ and gathered them in the tables as discrete functions of φ . In [67, Appendix B] we develop a simple formulae relating the terms $Q_n \alpha^n$ of the power series $\varepsilon_e(z)/\varepsilon_1$ to the terms $c_n z^n$

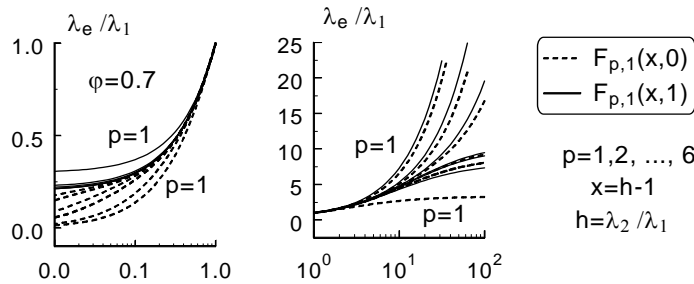


Fig. 4.8 Monotone sequence of upper and lower bounds evaluated from p coefficients of power expansion of $\lambda_e(x)$ uniformly converging to the effective conductivity $\lambda_e(x)$ of face-centered array of spheres.

of the power expansion of $\varepsilon_e(\alpha)/\varepsilon_1$. From the given coefficients Q_n [38, Tabs 6,7,8] we have calculated the unknown coefficients c_n . The T -continued fraction procedure (3.32)-(3.34) applied to $\sum_{n=1}^P c_n z^n$ yield the continued fraction coefficients g_n and constants w_P , gathered in Tab. 4.1. The sequence of the bounds $1+z\phi_{P,1}(z)$ or equivalently the inclusion regions $1+z\Phi_{P,1}(z)$, $P = 1, 2, 3, 4, 5, 6$ estimating the effective dielectric constants $\varepsilon_e/\varepsilon_1$ of regular arrays of spheres are shown in Figs 4.6 and 4.7. Note that the inclusion regions $z\Phi_{P,1}(z)$ satisfy the fundamental inclusion relations (4.17)-(4.18).

4.3.2 *Effective conductivity of regular arrays of spheres embedded in an infinite matrix [65]*

The results gathered in Table 4.1 were also applied to evaluate the bounds on the effective conductivity λ_e of simple, body-centered and face-centered, cubic lattices of spheres of a conductivity λ_2 embedded in an infinite matrix of the conductivity λ_1 . The calculation procedures used by us is reported in the Subsection 4.3.1. Results are shown in Fig. 4.8.

4.3.3 *Real dielectric constants of regular arrays of cylinders embedded in an infinite matrix [67].*

Let us consider square and hexagonal lattices of cylinders, with a dielectric constant ε_2 embedded in an infinite matrix made of a material with the dielectric coefficient ε_1 . By $\varepsilon_e(x)/\varepsilon_1$ ($x = h - 1$, $h = \varepsilon_2/\varepsilon_1$) we denote as previously the nondimensional effective dielectric constants of a composite. For a regular array of cylinders, the first two coefficients of power series expanded at zero are as follows

$$f_1(x) = \frac{\varepsilon_e(x) - \varepsilon_1}{x\varepsilon_1} = \varphi - \frac{1}{2}\varphi(1 - \varphi)x + O(x^2), \tag{4.79}$$

where $z = (\varepsilon_2/\varepsilon_1) - 1$. Here φ and $(1 - \varphi)$ denote the volume fractions of the cylinders and of the matrix, respectively. At $\xi = -1$ we can write

$$f_1(x) = 1 + O(x + 1). \tag{4.80}$$

Since $e_j = 0$ the T -continued fraction expansion of $f_1(z)$ is expressed by (cf. (4.79)-(4.80))

$$f_1(z) = \frac{\varphi}{1+x} \times \frac{\frac{1}{2}(1-\varphi)}{1+x} \times \frac{f_3(x)}{1}. \tag{4.81}$$

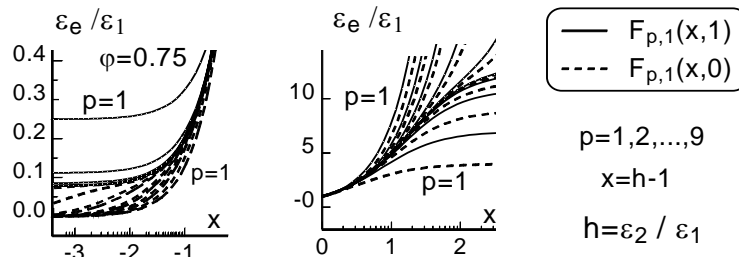


Fig. 4.9 The sequence of upper and lower bounds on the effective dielectric constant $\varepsilon_e(x)/\varepsilon_1$ of square array of cylinders.

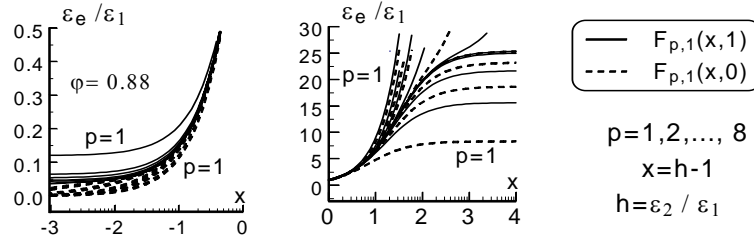


Fig. 4.10 The sequence of upper and lower bounds on the effective dielectric constant $\varepsilon_e(x)/\varepsilon_1$ of hexagonal array of cylinders.

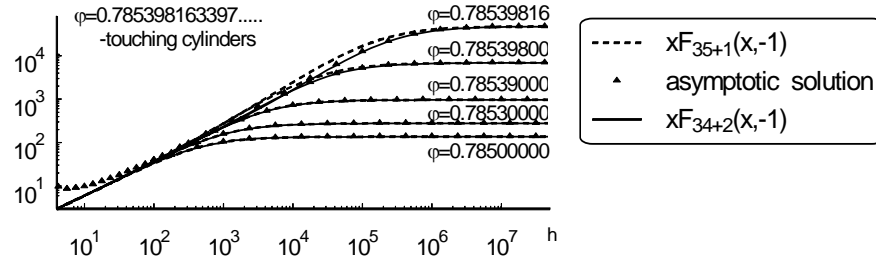


Fig. 4.11 Effective conductivity coefficients λ_e of a square array of nearly touching cylinders.

The low order bounding functions $xF_{P,1}(x, u)$, $p = 1, 2, 3$ (3.159) and the characteristic ones $R(x)$ (4.42) evaluated from (4.79) and (4.80) are given by (cf. (2.163))

$$\begin{aligned}
 xF_{1,1}(x, u) &= xF_1(x+1, u), \quad R(x) = H(x+1) + H(x), \\
 xF_{2,1}(z, u) &= x \frac{\varphi}{1+x} \times \frac{w_2 F_1(x+1, u)}{1}, \quad R(x) = H(x+1) + 2H(x), \\
 xF_{3,1}(x, u) &= x \frac{\varphi}{1+x} \times \frac{\frac{1}{2}(1-\varphi)x}{1+x} \times \frac{w_3 F_1(x+1, u)}{1}.
 \end{aligned} \tag{4.82}$$

Here $F_1(x, u) = 1 + u$, $-1 \leq u \leq 1$ is a real elementary bounding function, cf. (1.154). The relations (4.82_{1,2,5}) take the following explicit forms:

1) $P = 1$ – first coefficients of (4.80) is known

$$(-1)^{H(x+1)+H(x)} x \geq (-1)^{H(x+1)+H(x)} \left(\frac{\varepsilon_e}{\varepsilon_1} - 1 \right) \geq 0. \tag{4.83}$$

2) $P = 2$ – first coefficients of (4.80) and (4.79) are available

$$\begin{aligned}
 (-1)^{H(x+1)+2H(x)} x \frac{\varphi}{1+x} \times \frac{1-\varphi}{1} &\geq (-1)^{H(x+1)+2H(x)} \left(\frac{\varepsilon_e}{\varepsilon_1} - 1 \right) \geq \\
 &\geq (-1)^{H(x+1)+2H(x)} \frac{\varphi x}{1}.
 \end{aligned} \tag{4.84}$$

3) $P = 3$ – first coefficient of (4.80) and two coefficients of (4.79) are given

$$\begin{aligned}
 (-1)^{H(x+1)+3H(x)} x \frac{\varphi}{1+x} \times \frac{0.5(1-\varphi)}{1} &\geq (-1)^{H(x+1)+3H(x)} \left(\frac{\varepsilon_e}{\varepsilon_1} - 1 \right) \geq \\
 (-1)^{H(x+1)+3H(x)} x \frac{\varphi}{1+x} \times \frac{0.5(1-\varphi)}{1+x} \times \frac{0.5}{1}.
 \end{aligned} \tag{4.85}$$

Relations (4.84) and (4.85) are well known as the Wiener [73] and Hashin-Shtrikman bounds [30], respectively. The calculation of better bounds requires more than two coefficients of the power expansion of $(\varepsilon_e/\varepsilon_1) - 1$. For square and hexagonal arrays of cylinders, the terms c_n ($n = 1, 2, \dots, 6$) of the power expansion of $(\varepsilon_e/\varepsilon_1 - 1)/z$ have been calculated by the method presented in [37] and gathered in Table 4.2. The T -multipoint continued fraction procedure (2.13)-(2.14) applied to $\sum_{n=1}^P c_n x^n$ provides g_n , $n = 1, 2, \dots, P$ and w_P , $P = 1, 2, \dots, 7$, see Table 4.2. The narrowing sequences of the upper and lower bounds on the effective dielectric constants for square and hexagonal arrays of cylinders are shown in Figs 4.9 and 4.10, respectively.

4.3.4 *Densely packed highly conducting cylinders* [58, 59]

Let us consider an infinite array of identical, parallel cylinders arranged in a square lattice. Without loss of generality we assume that the nearest-neighbour distance at the cylinder axis is equal to one. We denote the cylinders radius by ϱ . The difference of the conductivities of the cylinders and the matrix medium is denoted by $x = h - 1$. The continuous temperature distribution in the system considered obeys the conductivity equations of the form

$$\nabla \cdot (1 + x\Theta_2)\nabla T = 0, \quad (4.86)$$

where Θ_2 is the characteristic function of the volume occupied by the cylinders. The conductivity equation (4.86) is supplemented by the continuity condition for the normal component of the heat current $\mathbf{J} = (1 + x\Theta_2)\nabla T$ at the surfaces of the cylinders.

In order to evaluate the effective heat conductivity we consider the system under the influence of a constant temperature gradient along one of the main square lattice axis, say in the X -direction. The temperature field can be then decomposed into the systematic part $T^{(0)}$ and the periodic part δT

$$T = T^{(0)} + \delta T. \quad (4.87)$$

Since the problem is linear the amplitude of the temperature field is irrelevant. Therefore we may set

$$T^{(0)} = X. \quad (4.88)$$

Also, since δT is periodic in space it is sufficient to consider the conductivity equation (4.86) in a single unit cell, with a periodic boundary condition for δT .

The effective conductivity coefficient λ_e is related to the above-defined temperature field by the following equation

$$\lambda_e = \left\langle (1 + x\Theta_2) \frac{\partial T}{\partial X} \right\rangle, \quad (4.89)$$

where $\langle \dots \rangle = S^{-1} \int_S \dots dS$ denotes the average over a unit cell.

The solution of (4.86)-(4.89) is obtained in the form of the power expansion

$$\frac{\lambda_e(x) - 1}{x} = \sum_{n=0}^{\infty} c_n x^n, \quad c_n = \pi g_1^{(n)} \varrho^2, \quad (4.90)$$

where $g_1^{(n)}$ is determined by

$$g_m^{(n+1)} = - \sum_{k=1}^{\infty} g_k^{(n)} \left(\frac{1}{2} \delta_{km} + a_{km} \frac{m \varrho^{k+m}}{2k!} \right), \quad g_m^{(1)} = \delta_{1m}, \quad (4.91)$$

$$a_{km} = (-1)^k \frac{(m+k)!}{m!} \left(A_{km} + \frac{1}{2} \pi \delta_{m+k,2} \right).$$

Table 4.3 Discrete values of the elastic torsional modulus $Q(X)/\mu_1 - 1$ for the hexagonal array of cylinders, after [46]

x	$\varphi=0.76$	$\varphi=0.80$	$\varphi=0.84$	$\varphi=0.88$
-1	-0.8711	-0.8996	-0.9286	-0.9607
0	0.0000	0.0000	0.0000	0.0000
9	3.3778	3.9489	4.6887	5.7225
49	5.7076	7.2600	9.7931	5.1565
∞	6.7600	8.9586	3.0093	24.4508

Here A_{km} denotes the coefficients of a Wigner potential evaluated in [46]. Several terms of the asymptotic expansion of λ_e at $x = \infty$ have been obtained by McPhedran and his collaborators [39]. Namely they have shown for nearly touching cylinders that

$$\lambda_e(x) - 1 = d_0 + d_1 \frac{1}{x} + O\left(\left(\frac{1}{x}\right)^{-2}\right), \quad d_0 = \pi(r-1), \quad d_1 = -2\pi r(r-1) \ln r, \quad (4.92)$$

where r is given by

$$r = \sqrt{\frac{\pi}{(\pi - 4\varphi)}}. \quad (4.93)$$

The two-point Padé approximants $xF_{35+1}(x, -1)$ and $xF_{34+2}(x, -1)$ to the truncated power series (4.90)-(4.93) were evaluated and depicted in Fig. 4.11. For volume fractions $\varphi = 0.7853$ and 0.78539 the lower $xF_{34+2}(x, -1)$ and upper $xF_{35+1}(x, -1)$ bounds are narrow, with the maximal difference of the order of 2%. Only for very high volume fraction, such as $\varphi = 0.785398$ and 0.78539816 the maximum difference between the bounds grows about 10% to 50%.

4.4 Complex torsional rigidity of a cancellous bone filled with a marrow [70]

4.4.1 Mathematical model of a prism-like cancellous bone.

Let us consider a two-phase material consisting of elastic porous solid filled with viscoelastic fluid. Such an idealized composite material is used to model a trabecular bone. Assume that $\lambda_1^* = \lambda_1' + i\lambda_1''$ and $\mu_1^* = \mu_1' + i\mu_1''$ are complex moduli of the solid phase, while $\lambda_2^* = \lambda_2' + i\lambda_2''$ and $\mu_2^* = \mu_2' + i\mu_2''$ characterize the viscoelastic properties of the fluid phase. Note that the case $\lambda_1'' = 0$, $\mu_1'' = 0$ and $\lambda_2' = 0$, $\mu_2' = 0$ represents a material consisting of a porous elastic matrix filled with a Newtonian fluid. For the oscillating viscoelastic solid-fluid composite the governing equations take the form

$$\overset{n}{\sigma}_{ij,j} = 0 \quad \text{on } \overset{n}{\Omega}, \quad n = 0, 1, \quad (4.94)$$

where

$$\overset{n}{\sigma}_{ij} = \lambda_n^* \overset{n}{u}_{k,k} \delta_{ij} + \mu_n^* \left(\overset{n}{u}_{i,j} + \overset{n}{u}_{j,i} \right) \quad \text{in } \overset{n}{\Omega}, \quad n = 1, 2. \quad (4.95)$$

The interface conditions are given by

$$\overset{1}{u}_i = \overset{2}{u}_i, \quad \overset{1}{\sigma}_{ij} m_j = \overset{2}{\sigma}_{ij} m_j \quad \text{on } \overset{1}{\partial\Omega}. \quad (4.96)$$

The boundary condition is classical

$$\overset{1}{\sigma}_{ij} m_j = g_i \quad \text{on } \overset{1}{\partial\Omega}. \quad (4.97)$$

Here σ_{ij}^1 , σ_{ij}^2 , u_i^1 and u_i^2 denote the components of stress and displacement fields in the solid and fluid phases respectively, while g_i are prescribed forces. The geometry of the composite material is defined by: Ω^1 is the domain occupied by a matrix, while Ω^2 denotes the domain occupied by fluid, $\Omega = \Omega^1 \cup \Omega^2$ is the domain occupied by a composite material, $\partial\Omega^1$ and $\partial\Omega^2$ are the surfaces enclosing the solid and fluid phases, respectively. As usual $\partial\Omega$ denotes the boundary of Ω , \mathbf{m} stands for the unit vector normal to $\partial\Omega^1$ and $\partial\Omega^2$ and is directed outwards.

4.4.2 Torsion of an inhomogeneous beam

Consider a porous beam filled with a fluid. Assume that at the opposite ends of the beam the torsional moments are applied. For such a case the displacement field takes the form [45]

$$u_1 = -\alpha X_3 X_2, \quad u_2 = \alpha X_3 X_1, \quad u_3 = \alpha \beta(X_1, X_2) \text{ in } \Omega = \Omega^1 \cup \Omega^2, \quad (4.98)$$

$$\sigma_{11} = \sigma_{22} = \sigma_{33} = \sigma_{12} = \sigma_{21} = 0 \text{ in } \Omega = \Omega^1 \cup \Omega^2. \quad (4.99)$$

The parameter α denotes the torsional angle of unit length of the beam. By substituting (4.98)-(4.99) to (4.94)-(4.97) we obtain

$$\sigma_{k3} = \alpha \Gamma^*(X) \frac{\partial}{\partial X_k} ((\beta(X) + (-1)^k X_k X_{k\pm 1})) \text{ in } \Omega, \quad k = 1, 2; \quad X = (X_1, X_2), \quad (4.100)$$

where

$$X_{k\pm 1} = \begin{cases} X_{k+1}, & \text{if } k = 1, \\ X_{k-1}, & \text{if } k = 2. \end{cases}, \quad \Gamma^*(X) = \Theta_1(X)\mu_1^* + \Theta_2(X)\mu_2^*. \quad (4.101)$$

Here $\Theta_i(X)$, $i = 1, 2$, are the characteristic functions: $\Theta_i(X) = 1$ ($\Theta_i(X) = 0$), if X belongs (does not belong) to the phase i . The stresses σ_{k3} given by Eq. (4.100) satisfy the equilibrium equation, cf. (4.100),

$$\sum_{k=1}^2 \frac{\partial}{\partial X_k} \left[\Gamma^*(X) \frac{\partial}{\partial X_k} (\beta(X) + (-1)^k X_k X_{k\pm 1}) \right] = 0 \text{ in } \Omega \quad (4.102)$$

and the interface condition

$$\sum_{k=1}^2 \Gamma^*(X) \frac{\partial}{\partial X_k} (\beta(X) + (-1)^k X_k X_{k\pm 1}) m_k = 0 \text{ on } \partial\Omega. \quad (4.103)$$

Here $\partial\Omega^l$ denotes the lateral surface of the beam, while $\Gamma^*(X)$ is the complex shear modulus. The set of equations (4.98)-(4.99) and (4.102)-(4.103) describe the torsional response of the prismatic solid-fluid beam under harmonically oscillating external moments.

4.4.3 Homogenization of an anisotropic inhomogeneous beam

In the sequel we restrict our considerations to a periodic distribution of shear modulus now represented by

$$\Gamma^*(X) = \Gamma^{*\varepsilon}(X) = \Gamma^*\left(\frac{X}{\varepsilon}\right), \quad (4.104)$$

where $\varepsilon > 0$ is a small, nondimensional parameter characterizing the periodicity of a cross-sectional microstructure of the porous beam.

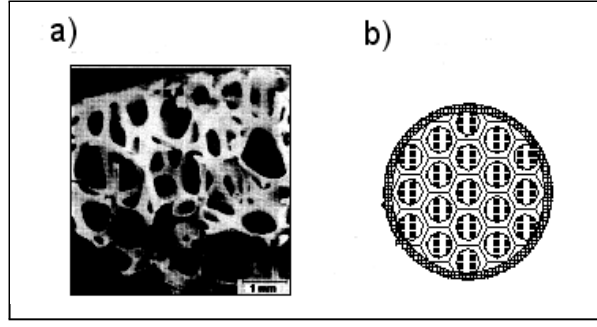


Fig. 4.12 (a) The scanning electron micrograph showing a prismatic structure of cancellous bone; a sample taken from the femoral head, after [23], pp. 318. (b) An idealized structural model of a prism-like cancellous bone represented by hexagonal array of fluid cylinders spaced in an elastic matrix.

Table 4.4 Multipoint Padé approximants $1 + [3/3]$ and $1 + [2/2]$ to torsional modulus $Q(X)/\mu_1$ of a hexagonal array of elastic cylinders embedded in an elastic beam; φ -volume fraction

φ	$1 + xF_{4+1}(x, 0)$	$1 + xF_{4+1}(x, -1)$
0.76	$\frac{1+1.7328x+0.9159x^2+0.1476x^3}{1+0.9728x+0.2678x^2+0.0190x^3}$	$\frac{1+1.3460x+0.4066x^2}{1+0.5860x+0.0524x^2}$
0.80	$\frac{1+1.8655x+1.0787x^2+0.1910x^3}{1+1.0655x+0.3063x^2+0.0192x^3}$	$\frac{1+1.3364x+0.3881x^2}{1+0.5364x+0.0390x^2}$
0.84	$\frac{1+1.8901x+1.0865x^2+0.1816x^3}{1+1.0501x+0.2717x^2+0.0130x^3}$	$\frac{1+1.3048x+0.3481x^2}{1+0.4648x+0.0249x^2}$
0.88	$\frac{1+1.8582x+1.0009x^2+0.1345x^3}{1+0.9782x+0.1929x^2+0.0053x^3}$	$\frac{1+1.2331x+0.2685x^2}{1+0.3531x+0.0106x^2}$

By substituting (4.104) into (4.102) one obtains

$$\sum_{k=1}^2 \frac{\partial}{\partial X_k} \left[\Gamma^* \left(\frac{X}{\varepsilon} \right) \frac{\partial}{\partial X_k} (\beta^\varepsilon(X) + (-1)^k X_k X_{k\pm 1}) \right] = 0 \text{ in } \partial\Omega. \quad (4.105)$$

To solve Eq. (4.104) the two-scale asymptotic method was applied. After tedious calculations we arrive at the following homogenized boundary value problem replacing the exact one (4.102)-(4.103)

$$\begin{aligned} \sum_{j=1}^2 \sum_{k=1}^2 Q_{jk}^* \frac{\partial^2}{\partial X_j \partial X_k} (f(X) + (-1)^j X_k X_{k\pm 1}) &= 0, \\ \sum_{k=1}^2 Q_{jk}^* \frac{\partial}{\partial X_k} (f(X) + (-1)^k X_k X_{k\pm 1}) m_k &= 0, \end{aligned} \quad (4.106)$$

where

$$Q_{jk}^* = \int_Y \Gamma^*(y) \left(\delta_{jk} - \frac{\partial \chi^k(y)}{\partial y_j} \right) dy \quad (4.107)$$

are the *homogenized* coefficients. The Y -periodic functions χ^k appearing in (4.107) satisfy the equations

$$\sum_{j=1}^2 A_0^{(j)} \chi^k(y) = \frac{\partial}{\partial y_k} \Gamma^*(y), \quad A_0^{(j)} = \frac{\partial}{\partial y_j} \left(\Gamma^*(y) \frac{\partial}{\partial y_j} \right). \quad (4.108)$$

By substituting into (4.108) and (4.107) $\chi^k(y) = y_k - T^k(y)$ we obtain

Table 4.5 The torsional moduli $Q(z)/\mu_1$ for the inhomogeneous beam filled with the viscous forming hexagonal array of cylinders: $Q(z)/\mu_1 = 1 + [3/3](z)$, $z = 1 - (I\omega/\varkappa)$, $\varkappa = \mu_1/\mu_2$; φ - the volume fraction

φ	$\frac{Q^*(z)}{\mu_1}, z = \frac{I\omega}{\varkappa} - 1, \varkappa = \frac{\mu_1}{\mu_2}$
0.76	$7.760 - \frac{60.980\varkappa}{10.09\varkappa - I\omega} - \frac{0.0974\varkappa}{4.157\varkappa - I\omega} - \frac{0.0431\varkappa}{2.831\varkappa - I\omega}$
0.80	$9.957 - \frac{102.62\varkappa}{12.56\varkappa - I\omega} - \frac{0.1831\varkappa}{3.814\varkappa - I\omega} - \frac{.0218\varkappa}{2.603\varkappa - I\omega}$
0.84	$14.01 - \frac{209.39\varkappa}{17.27\varkappa - I\omega} - \frac{0.4192\varkappa}{4.210\varkappa - I\omega} - \frac{0.0192\varkappa}{2.477\varkappa - I\omega}$
0.88	$25.45 - \frac{737.96\varkappa}{31.67\varkappa - I\omega} - \frac{1.6569\varkappa}{5.446\varkappa - I\omega} - \frac{.02234\varkappa}{2.388\varkappa - I\omega}$

$$Q_{jk}^* = \int_Y \Gamma^*(y) \frac{\partial T^k(y)}{\partial y_j} dy, \quad j, k = 1, 2. \quad (4.109)$$

Here $T^k(y)$ are determined by

$$\sum_{j=1}^2 \frac{\partial}{\partial y_j} \left(\Gamma^*(y) \frac{\partial T^k(y)}{\partial y_j} \right) = 0, \quad (y_k - T^k(y)) \quad Y - \text{periodic}. \quad (4.110)$$

Relations (4.109)-(4.110) with $\Gamma^*(y)$ given by (4.101) were investigated in Chapter 1 in the context of the effective transport coefficients of two-phase composite materials. Thus the torsional modulus $Q_{jk}^*(z)/\mu_1$ has a Stieltjes integral representation of the form (cf. (1.51))

$$\frac{Q_{jk}^*(z)}{\mu_1} - \delta_{jk} = z \int_0^1 \frac{d\beta_{jk}(v)}{1 + zv}, \quad z = \frac{\mu_2^*}{\mu_1^*} - 1, \quad (4.111)$$

where $\beta_{jk}(v)$ is a nonnegative-definite tensor.

Now let us consider an inhomogeneous beam consisting of cylinders regularly spaced in a solid phase and filled with a fluid. For such a porous beam we have $T^1 = T^2 = T$, $Q_{11}^* = Q_{22}^* = Q^*$ and $Q_{12}^* = Q_{21}^* = 0$, see Fig. 1b. On account of that the anisotropic boundary value problem (4.109)-(4.110) reduces to the isotropic one

$$Q^* = \int_Y \Gamma^*(y) \frac{\partial T(y)}{\partial y_1} dy, \quad (4.112)$$

where

$$\frac{\partial}{\partial y_1} \left(\Gamma^*(y) \frac{\partial T(y)}{\partial y_1} \right) + \frac{\partial}{\partial y_2} \left(\Gamma^*(y) \frac{\partial T(y)}{\partial y_2} \right) = 0, \quad (y_1 - T(y)) \text{ is } Y - \text{periodic}. \quad (4.113)$$

4.4.4 Hexagonal array of elastic cylinders

First we consider a hexagonal array of elastic cylinders embedded in an elastic matrix. For such a case the parameters μ_1^* , μ_2^* and consequently $z = \mu_2^*/\mu_1^* - 1$ take real values only. For convenience we set $Q^* = Q$, $\mu_1^* = \mu_1' = \mu_1$, $\mu_2^* = \mu_2' = \mu_2$ and $z = x$. From (4.111), it follows that the solution $Q(x)/\mu_1$ of the boundary value problem (4.112)-(4.113) has a

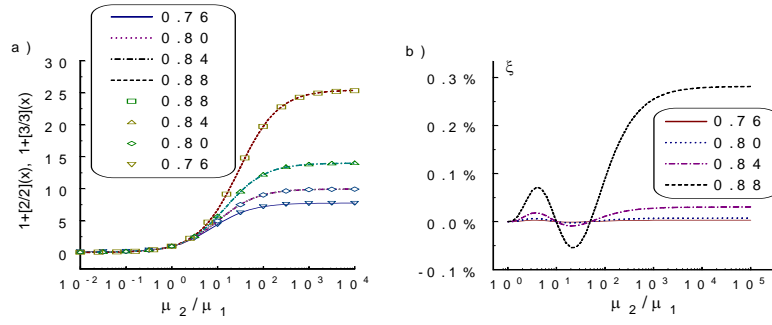


Fig. 4.13 Hexagonal array of elastic cylinders with volume fraction φ and physical parameter $x = (\mu_2/\mu_1) - 1$; (a) multipoint Padé bounds $1 + [3/3](x)$ (conventional lines) and $1 + [2/2](x)$ (scattered line) on the torsional modulus $Q(x)/\mu_1$, (b) error $\xi = 100\% \times \{[3/3](x) - [2/2](x)\} / \{1 + [3/3](x)\}$ for $Q(x)/\mu_1$.

Stieltjes integral representation

$$\frac{Q(x)}{\mu_1} - 1 = z \int_0^1 \frac{d\beta(v)}{1 + xv}, \quad x = \frac{\mu_2}{\mu_1} - 1. \quad (4.114)$$

In order to find $Q(x)/\mu_1$ by means of TCMFM the following informations are required:

- (i) The discrete values of $(Q(x)/\mu_1) - 1$ given for $\varphi = \varphi_j$ and $x = x_i$, see Tab. 4.3.
- (ii) The expansion of $((Q(x)/\mu_1) - 1)/x$ at $x = 0$: $(Q(x)/\mu_1) - 1 = \varphi + 0.5\varphi(1 - \varphi)x + O(x^2)$.

By starting from the input data (i) and (ii) the multipoint Padé approximants

$$1 + xF_{4+1}(x, 0) = 1 + [3/3](x) \quad \text{and} \quad 1 + xF_{4+1}(x, -1) = 1 + [2/2](x) \quad (4.115)$$

are evaluated and gathered in Table 4.4. The rational functions $1 + [3/3](x)$ and $1 + [2/2](x)$ estimate $Q(x)/\mu_1$ as follows (cf. (4.41))

$$(-1)^{R(x)} (1 + xF_{4+1}(x, 0)) \geq (-1)^{R(x)} Q(x)/\mu_1 \geq (-1)^{R(x)} (1 + xF_{4+1}(x, -1)), \quad (4.116)$$

$$R(x) = H(x + 1) + 3H(x) + H(x - 9) + H(x - 49) + H(x - \infty).$$

Fig. 4.13 depicts: a) the Padé bounds $1 + [3/3](x)$ and $1 + xF_{4+1}(x, -1)$ on torsional modulus $Q(x)/\mu_1$, b) the approximation error $\xi = 100\% \times \{[3/3](x) - [2/2](x)\} / \{1 + [3/3](x)\}$, $x = \mu_2/\mu_1 - 1$ for $Q(x)/\mu_1$. From Fig.4.13 we conclude that the torsional modulus $Q(x)/\mu_1$ differs from the multipoint Padé approximants $1 + [3/3](x)$ and $1 + [2/2](x)$ by less than 0.3%. On account of that we assume that the function

$$Q(x)/\mu_1 = 1 + [3/3](x), \quad x = (\mu_2/\mu_1) - 1, \quad \varphi \leq 0.88 \quad (4.117)$$

provides a good estimate of the effective torsional modulus.

4.4.5 Hexagonal array of fluid cylinders

Consider now a hexagonal array of cylinders filled with a viscous fluid and spaced in an elastic beam. For such a case the parameters μ_1^* , μ_2^* and consequently $z = \mu_2^*/\mu_1^* - 1$ take complex values. By replacing in (4.117) x by z one obtains the complex torsional modulus $Q^*(z)/\mu_1$ (cf. [16])

$$Q^*(z)/\mu_1 = 1 + [3/3](z) \quad \text{for} \quad \varphi \leq 0.88, \quad z = I\omega\mu_2/\mu_1 - 1. \quad (4.118)$$

Table 4.6 The torsional moduli $Q^{-1}(z)\mu_1$ for the porous beam filled with a viscous fluid forming hexagonal array of cylinders: $Q(z)/\mu_1 = 1 + [3/3](z)$, $z = 1 - (I\omega/\varkappa)$, $\varkappa = \mu_1/\mu_2$; φ - the volume fraction

φ	$\frac{\mu_1}{Q^*(z)}, z = 1 - \frac{I\omega}{\varkappa}, \varkappa = \frac{\mu_1}{\mu_2}$
0.76	$0.129 + \frac{0.0146\varkappa}{4.196\varkappa - I\omega} + \frac{0.0655\varkappa}{2.887\varkappa - I\omega} + \frac{0.9348\varkappa}{2.124\varkappa - I\omega}$
0.80	$0.100 + \frac{0.0476\varkappa}{3.911\varkappa - I\omega} + \frac{0.0666\varkappa}{2.643\varkappa - I\omega} + \frac{0.9226\varkappa}{2.095\varkappa - I\omega}$
0.84	$0.071 + \frac{0.07551\varkappa}{4.397\varkappa - I\omega} + \frac{0.0925\varkappa}{2.521\varkappa - I\omega} + \frac{0.9011\varkappa}{2.066\varkappa - I\omega}$
0.88	$0.039 + \frac{0.1339\varkappa}{5.956\varkappa - I\omega} + \frac{0.1471\varkappa}{2.450\varkappa - I\omega} + \frac{0.8608\varkappa}{2.034\varkappa - I\omega}$

Here μ_1 is the shear modulus of the elastic matrix, while μ_2 denotes the viscous coefficient of a Newtonian fluid. Tables 4.5 and 4.6 depicts formulae for complex moduli $Q^*(z)/\mu_1$ and complex compliances $\mu_1/Q^*(z)$, $z = (I\omega\mu_2/\mu_1) - 1$ of the hexagonal array of fluid cylinders. Figs 4.14 and 4.15 present a complex modulus $Q^*(z)/\mu_1$ and its real and imaginary parts, respectively.

Note that the modulus $Q^*(z)/\mu_1$ and compliance $\mu_1/Q^*(z)$, $z = (I\omega/\varkappa) - 1$, $\varkappa = \mu_1/\mu_2$ divided by $I\omega$ are Fourier transforms of torsional creep function $\Phi(t)$ and torsional relaxation function $\Psi(t)$, cf. [16]. Hence we can write

$$\mu_1 \overline{\Phi(I\omega)} = \frac{\mu_1}{I\omega Q^*(z)}, \quad \frac{\overline{\Psi(I\omega)}}{\mu_1} = \frac{Q^*(z)}{I\omega\mu_1}, \quad z = \frac{I\omega\mu_2}{\mu_1} - 1. \quad (4.119)$$

The inverse of the Fourier transformations of $\overline{\Phi(I\omega)}$ and $\overline{\Psi(I\omega)}$ are of the forms, cf. Tab. 4.5 and 4.6 and Eq. (4.119)

$$\begin{aligned} \mu_1 \Phi(t) &= d^c + \sum_{n=1}^3 \frac{b_n^c}{a_n^c} (1 - (1 + a_n^c \varkappa t) e^{-\varkappa t}), \\ \frac{\Psi(t)}{\mu_1} &= d^r - \sum_{n=1}^3 \frac{b_n^r}{a_n^r} (1 - (1 + a_n^r \varkappa t) e^{-\varkappa t}). \end{aligned} \quad (4.120)$$

Here the coefficients $d^c, d^r, b_n^c, b_n^r, a_n^c$ and a_n^r take values listed in Table 4.7 and Table 4.8.

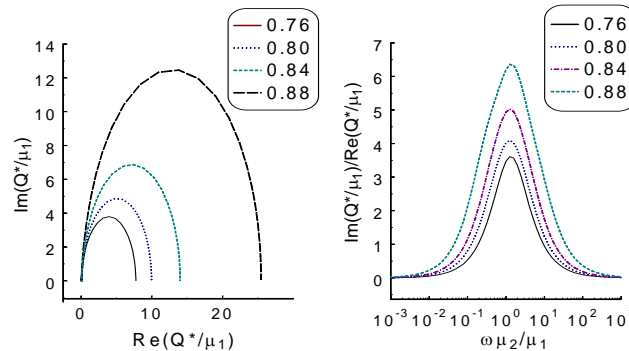


Fig. 4.14 Complex torsional modulus for the elastic beam filled with viscous fluid; $\varphi = 0.76, 0.80, 0.84, 0.88$.

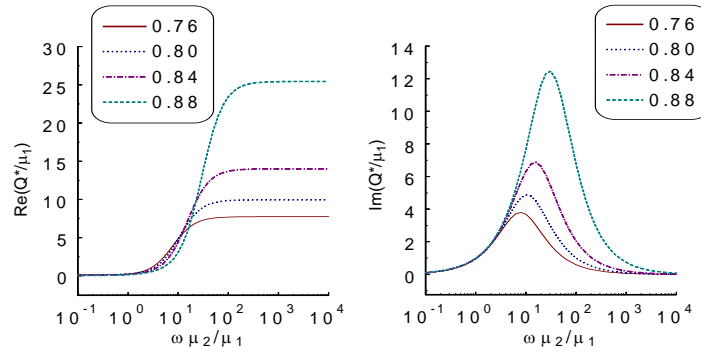


Fig. 4.15 Real and imaginary parts of the effective torsional moduli for the elastic beam filled with viscous fluid, $\varphi = 0.76, 0.80, 0.84, 0.88$.

Table 4.7

φ	d^c	b_1^c	b_2^c	b_3^c	a_1^c	a_2^c	a_3^c
0.76	0.1289	0.0146	0.0655	0.9348	2.1958	0.8867	0.1238
0.80	0.1004	0.0476	0.0666	0.9226	1.9109	0.6432	0.0948
0.84	0.0714	0.0755	0.0925	0.9011	2.3972	0.5213	0.0656
0.88	0.0393	0.1339	0.1471	0.8608	3.9565	0.4500	0.0344

Table 4.8

φ	d^r	b_1^r	b_2^r	b_3^r	a_1^r	a_2^r	a_3^r
0.76	7.7600	60.980	0.0974	0.0431	8.0939	2.1575	0.8312
0.80	9.9586	102.62	0.1831	0.0218	10.557	1.8143	0.6035
0.84	14.009	209.39	0.4192	0.0192	15.275	2.2101	0.4768
0.88	25.451	737.96	1.6569	0.0223	29.669	3.4456	0.3877

The torsional creep $\Phi(t)$ and relaxation $\Psi(t)$ functions given by (4.120) and Tables 4.7, 4.8 are depicted in Fig. 4.16

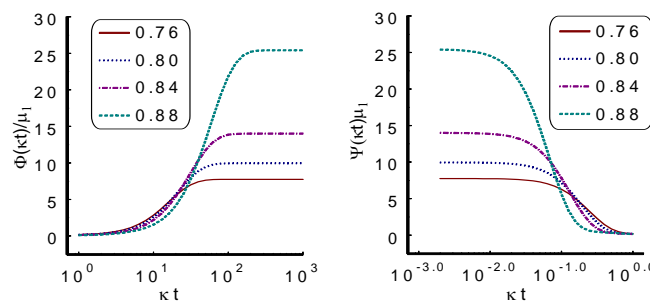


Fig. 4.16 The torsional creep function $\Phi(t)$ and torsional relaxation function $\Psi(t)$ for a porous beam consisting of hexagonal array of fluid cylinders spaced in a linear elastic matrix.

4.4.6 Torsional rigidity of prism-like cancellous bone

Most of bones in the body consists of a dense compact bone surrounding a spongy cancellous one filled with marrow, see 4.12. In previous sections the macroscopic torsional modulus, torsional creep function and torsional relaxation one have been evaluated for cancellous bone. Consider now a homogeneous viscoelastic material surrounded by an elastic one. Such a composite models a prism-like human bone, see Fig. 4.17. Two

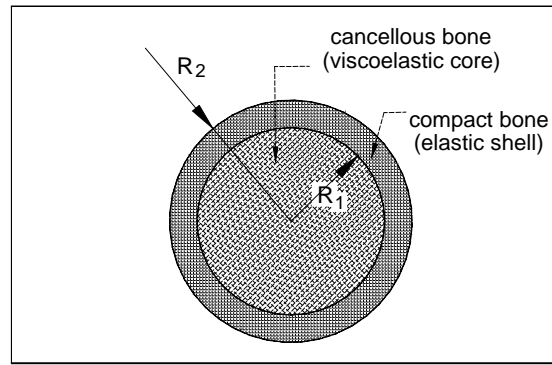


Fig. 4.17 An idealized model of typical human bone after the process of homogenization of a cancellous core.

equivalent relationships between the torsional angle α and torsional moment M are commonly used

$$\overline{\alpha(I\omega)} = I\omega \overline{\Phi^{ap}(I\omega)} \overline{M(I\omega)} \quad \text{or} \quad \overline{M(I\omega)} = I\omega \overline{\Psi^{ap}(I\omega)} \overline{\alpha(I\omega)}, \quad (4.121)$$

where

$$\frac{I\omega \overline{\Psi^{ap}(I\omega)}}{\mu_1} = \left(\int_{S_j} dx dy + \frac{I\omega \overline{\Psi(I\omega)}}{\mu_1} \int_{S_2} dx dy \right) \left(x^2 + y^2 + y \frac{\partial \overline{\beta(I\omega)}}{\partial x} - x \frac{\partial \overline{\beta(I\omega)}}{\partial y} \right). \quad (4.122)$$

Here $I\omega \overline{\Phi(I\omega)}$ and $I\omega \overline{\Psi(I\omega)}$ denote the torsional rigidity and torsional compliance of an inhomogeneous beam, respectively. The parameter μ_0 is the elastic modulus of the surrounding shell, while $I\omega \overline{\Psi(I\omega)}$ denotes the effective shear modulus of the viscoelastic core, cf. Fig. 4.17. For a circular cross-section (see Fig.4.17) we have $\beta(x, y, t) = 0$, thus $\beta(I\omega) = 0$. Formulae (4.121), (4.122) take the form

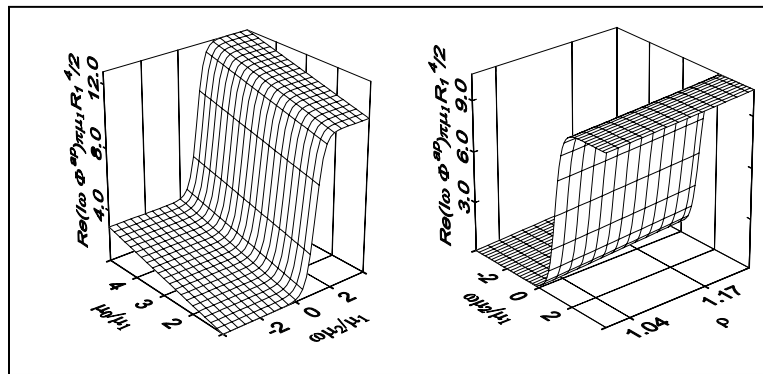


Fig. 4.18 The hydraulic stiffening of a torsional complex rigidity of a porous beam modelling a long human bone filled with marrow.

$$\frac{2I\omega \overline{\Psi^{ap}(I\omega)}}{\pi \mu_1 R_1^4} = \frac{\mu_0}{\mu_1} (\varrho^2 - 1) + \frac{I\omega \overline{\Psi^{ap}(I\omega)}}{\mu_1}, \quad \varrho = \frac{R_2^2}{R_1^2} \geq 1, \quad (4.123)$$

$$\frac{\pi R_1^4 \mu_1 I\omega \overline{\Phi^{ap}(I\omega)}}{2} = \frac{1}{\left(\frac{\mu_1}{\mu_0}\right)^{-1} (\varrho^2 - 1) + \frac{I\omega \overline{\Psi^{ap}(I\omega)}}{\mu_1}}, \quad \varrho = \frac{R_2^2}{R_1^2} \geq 1.$$

The influence of the parameter ϱ and ratios $\mu_0/\mu_1, \omega\mu_2/\mu_1$ on the nondimensional torsional rigidity $2I\omega \overline{\Psi^{ap}(I\omega)}/\pi \mu_1 R_1^4$ and nondimensional torsional compliance $\pi R_1^4 \mu_1 I\omega \overline{\Phi^{ap}(I\omega)}$ have been investigated. The results are depicted in Figs. 4.18 and 4.19.

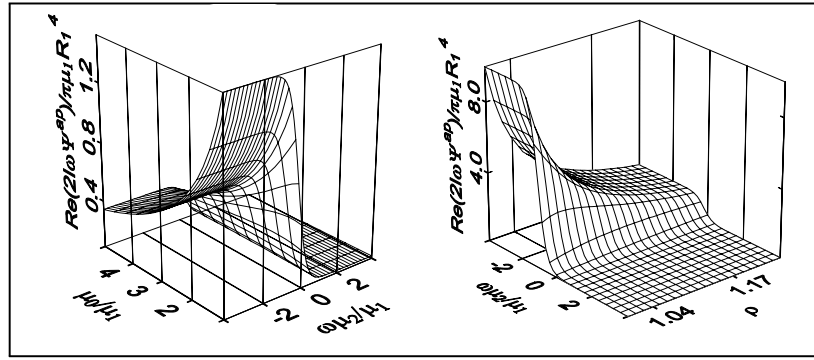


Fig. 4.19 The hydraulic stiffening of a torsional complex compliance of a porous beam modelling a long human bone filled with marrow.

4.4.7 Final remarks

In this study using TCMCFM we have developed an idealized model of a prism-like compact-cancellous bone structure filled with marrow. The model established predicts the mechanical response of prism-like cancellous structure loaded by torsional moments. The analytical formulae relating the torsional rigidity, compliance, creep and relaxation functions with apparent density, viscosity of marrow and elastic constants have been obtained. The formulae obtained predict the hydraulic stiffening of a human bone due the presence of a bone marrow.

4.5 Summary and final remarks about the TCMCFM estimates.

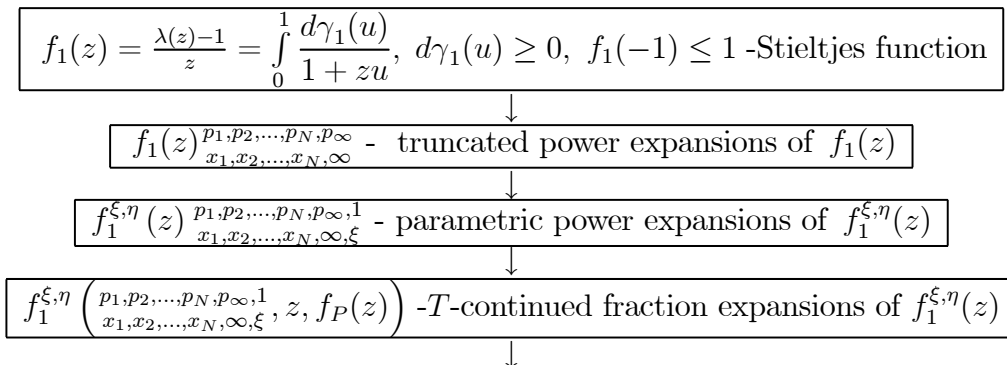
By means of TCMCFM established in the previous chapter we derive the general T -estimates of the effective transport coefficients $\lambda(z) - 1$ of two-phase media, namely the T -inclusion regions valid in a complex domain and the T -bounds defined on the real axes, cf. (4.19) and (4.51).

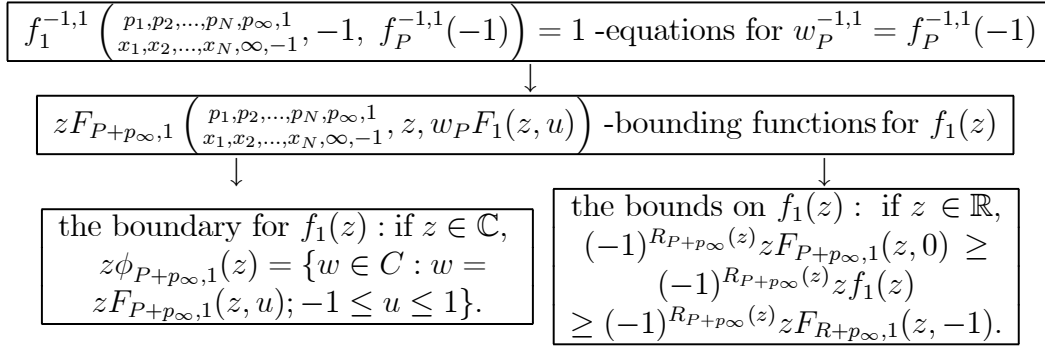
The fundamental T -estimates obtained are the optimum ones with respect to the given power series $(\lambda(z) - 1)/z$ available at real points (4.6), infinity (4.7) and satisfying the inequality (4.8).

The TCMCFM is a first method of the theory of composites materials that can incorporate into the estimates of the effective transport coefficients $\lambda(z) - 1$, among many others, also the power series $(\lambda(z) - 1)/z$ expanded at infinity.

The main TCMCFM tools adapted to composite materials, i.e. the fundamental T -inclusion relations (4.17)-(4.18) and the general T - inequalities (4.41)-(4.42) are new. They are published for the first time.

The following block diagram presents the TCMCFM computational steps for evaluating of the effective transport coefficients of two-phase media from the truncated power series





If in the above block diagram we replace z by s and $f_1(z)$ by $\varphi_1(s)$ we arrive at the TMC FM estimates of a Stieltjes function $\varphi_1(s) = \lambda(z) - 1$, $z = 1/s$, see Remark 3.2.

From the Subsections 4.1.1, 4.2.1 and the relations (4.19), (4.51), it follows that all previous bounds on $\lambda(z) - 1$ reported in literature [14, 42, 44, 53, 67] and [54, 58, 59] are the particular cases of the new T -estimates of $\lambda(z) - 1$ derived in this chapter.

As an examples of applications of the TMC FM we have investigated complex dielectric constants and termal conductivities of arrays of spheres, real dielectric constants of lattices of cylinders, conductivity coefficients for densely packed highly conducting cylinders and finally torsion rigidities of human bones filled with a marrow, see Sections 4.3.1, 4.3.2, 4.3.3, 4.3.4 and 4.4.

For more nontrivial examples of the estimations of complex material constants by means of TMC FM we refer the reader to our earlier papers exploring the effective transport properties of linear [3, 37, 60, 62, 64, 66, 68] and quasilinear [21, 22, 51, 57, 56] composites. In [52, 69] we also deal with effective torsional rigidities of long human bones filled with marrow.

CONCLUSIONS

By starting from the continued fraction techniques of matching up of the rational functions with the Stieltjes series developed by Baker [6, Chap.16, 17], [9, Chap. 5], Gilewicz [24], Gilewicz and Magnus [25, 26], Gilewicz *et al* [27], Tokarzewski [53, 54, 55] and Tokarzewski and Telega [66, 67, 68] we derived in a coherent form the new S - and T -Multipoint Continued Fraction Methods of an estimation of the effective transport coefficients $\lambda_e(z)/\lambda_1 - 1$ of two-phase media for the cases, where the inequality $[(\lambda_e(z)/\lambda_1) - 1]/z \Big|_{z=-1} \leq 1$ and the truncated power expansions of $(\lambda_e(z)/\lambda_1) - 1)/z$ at a number of real points (SMCFM) and infinity (TMC FM) are known. If no power expansion of $(\lambda_e(z)/\lambda_1) - 1)/z$ are given at infinity the TMC FM established in Chapter 3 reduces to the SMC FM derived in Chapter 2. On account of that we limit our further conclusions to TMC FM only.

The TMC FM is the first method of the mechanics of inhomogeneous media that incorporates into the complex and real estimates of $(\lambda_e(z)/\lambda_1) - 1$ the unlimited numbers of coefficients of power expansions of $(\lambda_e(z)/\lambda_1) - 1)/z$ available at a number of real points and infinity.

In the complex domain the TMC FM produces the T -multipoint inclusion regions (4.12) estimating via (4.17) the effective transport coefficients $(\lambda_e(z)/\lambda_1) - 1$ of two-phase media. They are optimal with respect to the truncated power expansions of $(\lambda_e(z)/\lambda_1) - 1)/z$ available at real points and infinity, see T -fundamental inclusion relations (4.17), Theorem 3.12 and Corollary 1.20.

In a real domain the T -multipoint inclusion regions (4.12) reduce to the segments lying on the real axis. The beginnings and the ends of these T - segments represent the optimal upper and lower multipoint Padé bounds on $(\lambda_e(z)/\lambda_1) - 1$ over the given numbers of coefficients of the power expansions of $(\lambda_e(z)/\lambda_1) - 1)/z$ at real points and infinity, see T -fundamental inequalities (4.41), Theorem 3.12 and Corollary 1.20.

On the basis of the relations (4.19)-(4.24) and (4.51)-(4.68) we conclude that TMC FM bounds generalize the classical estimates of $\lambda_e(z)/\lambda_1$ reported by Wiener [73], Hashin-Shtrikman [30], Milton [41, 40], Bergman [14] and the recent ones derived by Tokarzewski [53], Tokarzewski and Telega [67], Tokarzewski *et al* [58] and Telega *et al* [51].

It is worth adding that the SMC FM and TMC FM are new not only in mechanics of inhomogeneous media, but first of all in the theory of approximation of Stieltjes functions $f_1(z)$. Theorems 2.12 and 3.14 provide the best estimates of $f_1(z)$ from the power series expanded at real points and infinity.

Many nontrivial applications of the TMC FM are provided in this work. In Subsections 4.3.1 and 4.3.2 we compute the bounds on the complex dielectric constants $\epsilon_e(z)/\epsilon_1$ and effective conductivities $\lambda_e(x)/\lambda_1$ of simple-, body-, and face-centered cubic lattices of spheres, see Figs 4.6 and 4.8. In Subsections 4.3.3, 4.3.4 the real dielectric constants and thermal conductivities of square and hexagonal arrays of cylinders are studied, see Figs 4.9, 4.10 and 4.11. The torsional rigidity of a long human bone is investigated in Subsection 4.4, see Figs 4.18 and 4.19.

More examples of nontrivial applications of TMC FM provide our earlier papers dealing with the effective behaviors of natural and man-made two-phase media. In the articles [52, 69] the marrow influence on a complex rigidity of a long human bone is investigated. The papers [61, 63] deal with the complex dielectric constants of regular lattices of spheres, while [3, 37, 58, 60, 62, 64, 66, 68] and [21, 22, 51, 56, 57] explore the multipoint Padé bounds on the real effective conductivities of linear and quasilinear regular composites.

From the recurrence relations (3.32)-(3.34), it follows that the TMC FM is especially suited for an implementation as fast, accurate numerical algorithm, since it is recursive

and does not involve the solution of a large number of coupled equations or finding the zeros of a high-order polynomials.

It is worth noting that, while the bounds described in this contribution are optimal over the given input data, they are sometimes not optimal over the same input data. For example when the properties of constituents of composite are replaced by their reciprocals, then the effective coefficient obeys a certain "phase exchange inequality" [50] (in two dimension this become an equality [32]), which is violated by some of our bounds. It is therefore possible in those cases to get somewhat improved bounds on $\lambda_e(z)/\lambda_1$. Such a improved bounds are presented in [62].

It is commonly known [44, Chap.18, pp.422] that on the trajectories depending on one parameter the eigenvalues of the effective coefficients of linear composite materials have Stieltjes integral representations with a positive-semidefinite Stieltjes measures, cf. (1.51). Hence the TMCFM established in this contribution can also be applied to any linear inhomogeneous materials, for examples to viscous suspensions, porous materials, elastic and viscoelastic composites and media conducting heat and electrical currents.

The main aim of our future work is to extend the validity of TMCFM on the multi-components composite materials possessing anisotropic symmetries.

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