Multicomponent Composites, Electrical Networks and New Types of Continued Fraction II

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Abstract. The outstanding problem of systematically developing rigorous bounds on the complex effective conductivity tensor σ^* of d-dimensional, n-component composites with $n > 2$ is solved. The bounds incorporate information contained in successively higher order correlation functions which reflect the composite geometry. Explicit expressions are given for many of the bounds and some, but not all of them, are represented by nested sequences of circles in the complex plane that enclose, and in fact converge to, each diagonal element of σ^*. They are derived from the fractional linear matrix transformations found in Part I that recursively link σ^* with a hierarchy of complex effective tensors $\Omega^{(j)}$, $j = 0, 1, 2, \ldots$, of increasing dimension, $d(n-1)^j$. Elementary bounds on $\Omega^{(j)}$ confining the diagonal elements of $\Omega^{(j)}$ or its inverse to half-plane, wedge or open polygon regions of the complex plane, imply narrow bounds on σ^* which converge to the exact value of σ^* in the limit as $j \to \infty$. When the component conductivities are real these bounds are more restrictive than the corresponding variational bounds. Besides applying to the effective conductivity σ^*, the bounds extend to a wide class of matrix-valued multivariate functions called Ω-functions, and thereby to conduction in polycrystalline media, viscoelasticity in composites, and conduction in multi-component, multiterminal, linear electrical networks. The analytic and invariance properties of Ω-functions are explored and within this class of function most of the bounds are found to be optimal or at least attainable. The bounds obtained here are essentially a generalization to matrix-valued, multivariate functions of the nested sequence of lens-shaped bounds in the complex plane derived by Gragg and Baker for single variable Stieltjes functions.

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1. Introduction

The average current $\mathbf{j}$ generated in response to an average electric field $\mathbf{e}$ in a periodic or statistically homogeneous composite is typically determined by the linear relation

$$\mathbf{j} = \sigma^* \mathbf{e}, \tag{1.1}$$

which defines the effective conductivity tensor σ^*. In Part I [1], henceforth denoted as I, we considered a d-dimensional multicomponent composite comprised of n isotropic components separated by sharp boundaries and developed a continued fraction expansion for σ^* in terms of the component conductivities, $\sigma_1, \sigma_2, ..., \sigma_n$ and a sequence of geometric parameters that reflect successively finer details of the microstructure. Here this expansion will be utilized to solve an outstanding problem for composites comprised of more than two components, namely to systematically develop a hierarchy of bounds on σ^* that include progressively more information about the geometry, for both real and complex component conductivities. Actually our analysis is quite general and applies to the effective thermal conductivity, diffusion coefficient, dielectric, elastic and viscoelastic tensors of multicomponent composites, including polycrystalline materials with anisotropic grains [2]. Moreover it extends to conduction in multicomponent, multiterminal networks, and in fact to any problem for which the field equation has the appropriate form: see Sect. 15 in I.

The earliest work on bounds for effective transport coefficients dates back to Wiener [3] who in 1912 proved that the eigenvalues of σ^* are bounded above and below by the arithmetic and harmonic means of the local conductivity when the local conductivity is real. Not much more progress was made until half a century later when Hashin and Shtrikman [4] formulated new variational principles and used them to derive bounds on the effective conductivity, σ^*, of isotropic composites with real component conductivities, $\sigma_1, \sigma_2, ..., \sigma_n$. Their bounds proved to be considerably tighter than the Wiener bounds yet still were in excellent accord with experiment and only incorporated the component conductivities and volume fractions.

Beran [5] and Kröner [6], among others, went further and developed a scheme for generating a whole hierarchy of bounds which include information contained in successively higher order correlation functions characterizing the composite geometry. Improvements of these bounds for multicomponent composites (containing more than two components) were obtained by Phan-Thien and Milton [7]. The improved bounds are denoted in I as $(2j+1)$th-order Wiener-Beran bounds or $(2j)$th-order Hashin-Shtrikman bounds where $j = 0, 1, 2, ...$ signifies the order of the trial fields that generate the bounds: these fields are ranked according to their order of appearance in perturbation expansions of the actual fields in powers of the conductivity differences $\sigma_a - \sigma_b$, where $a, b \in \{1, 2, ..., n\}$.

Prager [8] considered two component composites and established bounds that correlate the values of σ^* at different conductivity ratios σ_1/σ_2. Willis [9] gave specific attention to anisotropic composites, and Murat and Tartar [10] and Lurie and Cherkaev [11] implemented the method of compensated compactness (which is essentially a new variational method with matrix valued fields) to obtain

realizable bounds correlating the different eigenvalues of σ^*. Kohn and Milton [12, 13] rederived these bounds and generalized them to elasticity by using the standard Hashin-Shtrikman variational principles. Such bounds have application in design optimization problems [14, 15].

Bergman [16] initiated a different approach. He considered any diagonal element, say σ^*_{11}, of the effective conductivity tensor of a two component composite with volume fractions f_1 and f_2 of the components and esssentially proved that the function $F(s)$, where

$$F \equiv 1 - \sigma^*_{11}/\sigma_2 \quad \text{and} \quad s \equiv \sigma_2/(\sigma_2 - \sigma_1), \tag{1.2}$$

satisfies the inequality

$$F(1) \leqq 1, \tag{1.3}$$

has the integral representation

$$F(s) = \int_0^1 \frac{\mu(z)\,dz}{s - z}, \quad \text{where} \quad \mu(z) \geqq 0, \tag{1.4}$$

and can be expanded in a series of the form

$$F(s) = f_1/s + c_2/s^2 + c_3/s^3 + c_4/s^4 + \dots, \tag{1.5}$$

in which $c_2 = f_1 f_2/d$ when the composite is isotropic: see also [17] and [18]. From this representation Bergman rederived the Hashin-Shtrikman bounds and obtained new Prager type bounds incorporating one known value of σ^*_{11} at any given real ratio $\sigma_1/\sigma_2 > 0$.

Subsequently, and independently, Bergman [19] and Milton [20], generalized the Wiener and Hashin-Shtrikman bounds to arbitrary complex ratios σ_1/σ_2 and proved that σ^*_{11} is confined to one of three nested lens-shaped inclusion regions in the complex plane, depending on whether the volume fractions are known, or whether the composite is isotropic. These results enlarge upon the variational bounds of Schulgasser and Hashin [21] which are valid when σ_1/σ_2 is nearly real. Complex conductivities, of course, are appropriate for describing the relation between $\mathbf{j}$ and $\mathbf{e}$, including the phase lag, when the applied fields oscillate but have wavelengths and attenuation lengths much larger than the composite inhomogeneities.

Following this work, the bounds were extended to encompass an arbitrary number of coefficients in the series expansion and/or an arbitrary number of known values of $\sigma^*_{11}(\sigma_1, \sigma_2)$ at either real or complex ratios σ_1/σ_2 [22]. McPhedran and Milton [23] numerically tested the bounds and together with McKenzie used them as a basis of a successful method [24] to estimate the volume fraction f_1 from experiments of the refractive index and absorption coefficient at various frequencies of the applied field. Gajdardziska-Josifovska [25] made a careful experimental test of the method and considered its applicability to composites with more than two components. Felderhof [26], Milton and Golden [27], and Golden [28] reformulated and analyzed the structure of the subset of bounds that only include series expansion coefficients, and Milton and McPhedran [29] proved their equivalence, for real σ_1 and σ_2, to the complete hierarchy of odd and even order

variational bounds, i.e. to the $(2j+1)$th-order Wiener-Beran bounds and $(2j)$th-order Hashin-Shtrikman bounds for $j = 0, 1, 2, \ldots$.

Additional assumptions about the analytic properties of $\sigma_{11}^*(\sigma_1, \sigma_2)$, which apply to certain classes of composites, produce even more restrictive bounds. For instance, Keller's duality relationship [30],

$$\sigma_{11}^*(1/\sigma_1, 1/\sigma_2) = 1/\sigma_{11}^*(\sigma_1, \sigma_2), \tag{1.6}$$

satisfied by the effective conductivity of isotropic two-dimensional composites, and the identity

$$\sigma_{11}^*(\sigma_1, \sigma_2) = \sigma_{11}^*(\sigma_2, \sigma_1), \tag{1.7}$$

appropriate to materials invariant under phase interchange, give substantial improvements to the bounds [20, 22, 31, 32]. In fact any bound in the double hierarchy of bounds [22] incorporating (1.6), an arbitrary number of known real or complex values of $\sigma_{11}^*(\sigma_1, \sigma_2)$, and an arbitrary number of series expansion coefficients is realizable by the transverse effective conductivity of a Hashin-Shtrikman type multicoated cylinder geometry [4]. Bergman [19] used Schulgasser's inequality [33] to marginally improve one arc of the complex extension of the Hashin-Shtrikman bounds in dimensions $d \geq 3$. Korringa and LaTorrica [34] incorporated information about $F(s)$ in the vicinity of $s = 0$, and utilized their bounds to analyze measurements of σ_{11}^* for brine saturated sandstones.

These and other contributions to the theory of bounds for two-component composites are reviewed by Hashin [35], McPhedran and Phan-Thien [36], Willis [37], McCoy [38], Christensen [39], Watt et al. [40], Hale [41], and Beran [42]: see also Niklasson and Granquist [43], Torquato and Stell [44] and references therein. Many of the developments, particularly including the results outlined above, overlap with work on Stieltjes functions [45–50]. To see the connection consider the function $\hbar(v)$, where

$$v \equiv -1/s = (\sigma_1 - \sigma_2)/\sigma_2 \quad \text{and} \quad \hbar(v) \equiv -F(v)/v = (\sigma_{11}^* - \sigma_2)/(\sigma_1 - \sigma_2). \tag{1.8}$$

From (1.4) this function has the integral representation

$$\hbar(v) = \int_0^1 \frac{\mu(z)\,dz}{1 + vz}, \tag{1.9}$$

which according to Baker and Graves-Morris [51] defines a Stieltjes function with a series expansion

$$\hbar(v) = f_1 - c_2 v + c_3 v^2 - c_4 v^3 + \ldots, \tag{1.10}$$

convergent in the unit disk.

Nevanlinna [45, 46] considered the more general class of Hamburger functions, which include Stieltjes functions, and found bounds which confine $\hbar(v)$ to a nested sequence of diskshaped inclusion regions in the complex plane as successively more series expansion coefficients are incorporated in the bounds. Henrici and Pfluger [47] used the well-known continued fraction expansion of Stieltjes functions, such as $\hbar(v)$, to derive a hierarchy of improved, and in fact

optimal, bounds for real and complex v which incorporate the series coefficients up to successively higher orders in v. Gragg [48] focussed on Stieltjes functions convergent in the unit disk and obtained more restrictive bounds, again based on a continued fraction expansion of $\hbar(v)$. Following earlier work of Common [49], Baker [50] also independently established these results and obtained bounds that in addition incorporate known values of $\hbar(v)$ at an arbitrary number of real values of v. All of the bounds are optimal within the appropriate class of Stieltjes functions and are represented by nested sequences of lens-shaped inclusion regions in the complex plane. While Gragg and Baker did not incorporate in their bounds the inequality

$$\hbar(-1) \leqq 1 , \qquad (1.11)$$

implied by (1.3) and (1.8), it is clear that if a bound depends on this inequality, then all functions that attain the bound have $\hbar(-1) = 1$, and this can be treated as a known value of $\hbar(v)$ for the purpose of calculating the bound in question. Suitable combinations of Gragg's bounds and Baker's bounds thereby yield the whole sequence of Wiener-Beran and Hashin-Shtrikman bounds, Prager's bounds, and many of the complex extensions of these bounds obtained by Bergman and Milton. The bounds derived for two-component composites go beyond the Gragg-Baker bounds to the extent that they incorporate known values of $\hbar(v)$ at complex v and (when appropriate) the functional relations on $\hbar(v)$ implied by (1.6) and (1.7). For a comprehensive review of work on bounds on Stieltjes functions, including their derivation for real v from variational principles and their connection with Páde approximants, see Baker and Graves-Morris [51] and Jones and Thron [52].

Very little of this analytical work on bounds has been generalized to composites with more than two components, or to multivariate Stieltjes functions. In Bergman's trajectory method [16] all the component conductivities are parameterized in terms of a single variable, say s. The parametrization is chosen so that the representation for $F(s)$ has the form (1.4), and then bounds on such functions imply bounds on σ_{11}^*. Using this approach Bergman rederived the Hashin-Shtrikman bounds for three component composites. Although the method has been quite successful, the best parametrization is often difficult to find and the method only incorporates the analytic properties of $\sigma_{11}^*(\sigma_1, \sigma_2, \ldots, \sigma_n)$ along a single trajectory in the full domain of the variables $\sigma_1, \sigma_2, \ldots, \sigma_n$. A multivariate generalization of the representation (1.4) was formulated by Golden and Papanicolaou [28, 53]. They used it to conjecture complex extensions of the elementary Wiener and Hashin-Shtrikman bounds, based on the plausible (but unproven) assertion that functions attaining elementary bounds should have especially simple representations after suitable fractional linear transformations. Subsequently, Bergman and Milton [54] extended the trajectory method to complex component conductivities and gave a rigorous proof of the Golden-Papanicolaou extensions of the Wiener bounds.

The main barrier to the development of bounds on σ^* for multicomponent composites when the conductivities $\sigma_1, \sigma_2, \ldots, \sigma_n$ are complex has been the lack of a suitable continued fraction expansion for σ^*. Now that several such expansions are available, the path is open to generalize the nested hierarchy of lens-shaped bounds appropriate for two-component composites to multicomponent composites.

The paper is structured as follows. In Sect. 2 we summarize most of the results obtained in I. These include recursion relations which link σ^* with a sequence of matrices $\Omega^{(j)}$, $j = 0, 1, 2, \ldots$, each representing the effective tensor in an appropriate Hilbert space, although not necessarily in a composite. Such effective tensors depend on the variables $\sigma_1, \sigma_2, \ldots, \sigma_n$ and are collectively denoted as n-variable tensor Ω-functions. Their general analytic and invariance properties are studied in Sect. 3. For instance it is proved that the diagonal elements of any tensor Ω-function are scalar Ω-functions.

Section 4 focuses on hierarchies of bounds for Ω-functions. Elementary restrictions on the diagonal elements of $\Omega^{(j)}$, for $j = 1, 2, \ldots$, to half-plane, wedge or open polygon regions of the complex plane, generate nested sequences of bounds on $\sigma^* = \Omega^{(0)}$: these are accordingly denoted as half-plane, wedge or polygon bounds. A bound here is defined to be *attainable* if at least some points on the boundary are attained by Ω-functions in the appropriate class, *optimal* if all points within the bounds are attainable by Ω-functions, and *realizable*, if all points within the bounds are realized by the effective conductivity tensor of a composite in the appropriate class. In terms of the information they contain, the half-plane bounds are attainable and the wedge bounds optimal for both real and complex σ_a, $a = 1, 2, \ldots, n$, at all levels in the hierarchy of bounds. When the conductivities σ_a are real both the wedge and polygon bounds are optimal and generally improve upon, or at worst coincide with, the hierarchy of Wiener-Beran and Hashin-Shtrikman variational bounds. The question of realizability of these bounds will be left for later work. For two-dimensional, two-component anisotropic composites we generalize the Murat, Tartar, Lurie and Cherkaev bounds [10, 11] to include successively higher order geometric parameters.

In Sect. 5 the mapping which links σ^* with $\Omega^{(j)}$ is proved to be a fractional linear matrix transformation. Section 6 utilizes this fact to derive explicit analytical expressions for the complete hierarchy of half-plane bounds on scalar multivariate Ω-functions. The inclusion regions are simply nested sequences of circles in the complex plane for each orientation of the half-plane. Section 7 identifies characteristics of the set of matrices that get mapped to the boundary of the wedge bounds and this should make numerical computations of the wedge bounds more efficient. An analytic formula is obtained for the curve needed in conjunction with the Golden-Papanicolaou bounds to complete the boundary of the 1st-order wedge bounds on scalar 3-variable Ω-functions. These bounds have direct practical importance because they only incorporate the volume fractions and conductivities in a three component composite: they are the complex extensions of the Wiener bounds. The convergence of the various hierarchies of bounds is established in Sect. 8.

2. Summary of Part I

Now let us review the results established in I. These apply in any Hilbert space

$$\mathcal{H}' = \mathcal{U} \oplus \mathcal{E}' \oplus \mathcal{J}' = \mathcal{P}'_1 \oplus \mathcal{P}'_2 \oplus \mathcal{P}'_3 \oplus \ldots \oplus \mathcal{P}'_n$$

of fields, where the subspaces $\mathcal{U}$, $\mathcal{E}'$, $\mathcal{J}'$, and $\mathcal{P}'_a$ are each invariant under complex conjugation, and $\mathcal{U}$ has finite dimension, d. Specifically, in a periodic composite

comprised of n isotropic components we may take $\mathscr{U}$ as the set of uniform applied fields, $\mathscr{E}'$ as the fluctuating periodic electric fields (that have zero average), $\mathscr{J}'$ as the fluctuating periodic current fields (with zero average), and $\mathscr{P}_a'$ as the periodic polarization fields that are non-zero only inside component a. Of course, other choices of these subspaces will be appropriate for conduction in polycrystalline media, conduction in multiterminal multicomponent impedance networks, and for viscoelasticity in composites: see Dell'Antonio et al. [2] and Sect. 15 in I. We let x_ℓ, $\ell = 1, 2, ..., d$, label an orthogonal basis set of fields for $\mathscr{U}$ and we let $\Gamma_0, \Gamma_1, \Gamma_2$, and χ_a denote the projection operators onto the subspaces $\mathscr{U}, \mathscr{E}', \mathscr{J}'$, and $\mathscr{P}_a'$. These projection operators, of course, satisfy the relations

$$\Gamma_i \Gamma_j = \delta_{ij} \Gamma_i, \quad \sum_{i=0}^{2} \Gamma_i = I, \chi_a \chi_b = \delta_{ab} \chi_a, \quad \sum_{a=1}^{n} \chi_a = I, \tag{2.1}$$

in which I is the identity operator in $\mathscr{H}'$. In general, the operators Γ_i do not commute with any of the operators χ_a.

In this Hilbert space the solutions $\mathbf{E}^* \in \mathscr{E}'$ and $\mathbf{J}^* \in \mathscr{J}'$ to the field equation of interest,

$$|\mathbf{j} + \mathbf{J}^*\rangle = \sum_{a=1}^{n} \sigma_a \chi_a |\mathbf{e} + \mathbf{E}^*\rangle, \tag{2.2}$$

for any $\mathbf{e} \in \mathscr{U}$ giving some $\mathbf{j} \in \mathscr{U}$ can be expanded in the set of real-valued fields $\mathbf{E}_\tau^0$ and $\mathbf{J}_\tau^0$ generated via the recursion relations,

$$
\begin{aligned}
|\mathbf{E}_{a\ell}^0\rangle &= \Gamma_1 \chi_a |\mathbf{x}_\ell\rangle, & |\mathbf{E}_{a\tau}^0\rangle &= \Gamma_1 \chi_a |\mathbf{E}_\tau^0\rangle, \\
|\mathbf{J}_{a\ell}^0\rangle &= \Gamma_2 \chi_a |\mathbf{x}_\ell\rangle, & |\mathbf{J}_{a\tau}^0\rangle &= -\Gamma_2 \chi_a |\mathbf{J}_\tau^0\rangle,
\end{aligned}
\tag{2.3}
$$

where $\ell = 1, 2, ..., d$ represents a direction index; $a = 1, 2, ..., n$ represents a component index; and $\tau = b\ell, bc\ell, ...$ represents a string of component indices followed by a single direction index.

To avoid confusion, *italic subscripts* ($\neq i, j$ or h) are reserved for component indices, *script subscripts*, such as ℓ, k, and m, represent direction indices, and *Greek subscripts* stand for strings of indices: the subscripts α and β signify strings of component indices while all other Greek subscripts represent a string of component indices followed by a direction index. We adopt the summation convention that *sums over repeated Greek or script subscripts are implied, while sums over repeated italic subscripts are not implied*. Given any string τ or α we let $o(\tau)$ and $o(\alpha)$ denote the number of component indices they contain, which we define as the *order of the string*.

As τ varies over all strings these fields $\mathbf{E}_\tau^0$ and $\mathbf{J}_\tau^0$ span subspaces $\mathscr{E} \subset \mathscr{E}'$ and $\mathscr{J} \subset \mathscr{J}'$. From (2.1) and (2.3) the fields satisfy

$$\sum_{b=1}^{n} \mathbf{E}_{\alpha b\omega}^0 = \mathbf{E}_{\alpha\omega}^0, \quad \sum_{b=1}^{n} \mathbf{J}_{\alpha b\omega}^0 = -\mathbf{J}_{\alpha\omega}^0, \tag{2.4}$$

where the sum extends over any component index in the string $\tau = \alpha b\omega$. This linear dependence allows us to choose one of the components as a *reference medium*, labelled as component $q \in \{1, 2, ..., n\}$, and eliminate those fields $\mathbf{E}_\tau^0$ and $\mathbf{J}_\tau^0$ for which τ contains a component index q to obtain natural basis sets for $\mathscr{E}$ and $\mathscr{J}$: see

for example Phan-Thien and Milton [7]. In some special circumstances, such as when $\mathscr{H}'$ has finite dimension, the fields obtained are still linearly dependent. To avoid prolonged discussion, this complication is tentatively overlooked.

Similarly, the polarization fields $\mathbf{P}_{a\tau}^0$ generated recursively via

$$|\mathbf{P}_{a\ell}^0\rangle = \chi_a|x_\ell\rangle, \qquad |\mathbf{P}_{a\tau}^0\rangle = \chi_a\Gamma_1|\mathbf{P}_\tau^0\rangle \tag{2.5}$$

span some subspace $\mathscr{P}_a \subset \mathscr{P}_a'$ and may (generally) be used as a basis set once we exclude those fields $\mathbf{P}_{a\tau}^0$ that have a component index with the value q in the string τ. Note this does not exclude the fields $\mathbf{P}_{q\tau}^0$ which span $\mathscr{P}_q$.

The need for alternative basis sets for $\mathscr{E}$, $\mathscr{J}$, and $\mathscr{P}_a$ arises because the fields $\mathbf{E}_\tau^0$, $\mathbf{J}_\tau^0$, and $\mathbf{P}_{a\tau}^0$ do not have any special orthogonality properties. In I, by using Gram-Schmidt orthogonalization followed by appropriate linear transformations, we obtain new sets of basis fields $\mathbf{E}_\tau'^{(q)}$, $\mathbf{J}_\tau'^{(q)}$, and $\mathbf{P}_{a\tau}'^{(q)}$ (where τ ranges over all strings not containing any component index equal to q). Their inner products

$$U_{\lambda,\eta}'^{(q)} \equiv \langle \mathbf{E}_\lambda'^{(q)}|\mathbf{E}_\eta'^{(q)}\rangle, \qquad V_{\lambda,\eta}'^{(q)} \equiv \langle \mathbf{J}_\lambda'^{(q)}|\mathbf{J}_\eta'^{(q)}\rangle, \qquad W_{a,\lambda,\eta}^{(q)} \equiv \langle \mathbf{P}_{a\lambda}'^{(q)}|\mathbf{P}_{a\eta}'^{(q)}\rangle \tag{2.6}$$

are block diagonal matrices, i.e. zero unless $o(\lambda) = o(\eta)$, and satisfy the relations

$$U' + V' = I, \qquad \sum_{a=1}^n W_a = I, \tag{2.7}$$

in which I is the identity matrix. Furthermore, the fields $\mathbf{x}_\omega^{(q)}$ and $\mathbf{y}_\tau^{(q)}$ defined by

$$\mathbf{x}_\omega^{(q)} = \sum_{a=1}^n \mathbf{P}_{a\omega}'^{(q)}, \qquad \mathbf{y}_\tau^{(q)} = \mathbf{E}_\tau'^{(q)} + \mathbf{J}_\tau'^{(q)}, \tag{2.8}$$

form an orthonormal basis set, denoted as a canonical basis set, for the Hilbert space

$$\mathscr{H} = \mathscr{U} \oplus \mathscr{E} \oplus \mathscr{J} = \mathscr{P}_1 \oplus \mathscr{P}_2 \oplus \ldots \oplus \mathscr{P}_n. \tag{2.9}$$

The *weight matrices* $W_a, a = 1, 2, \ldots, n$ defined via (2.6), together with the *normalization matrix* $N = N_{\lambda,\eta}^{(q)}$ defined by

$$N = (U')^{-1} - I = [(V')^{-1} - I]^{-1} \tag{2.10}$$

are positive-semidefinite matrices that, in fact, contain all the information necessary to calculate the effective tensor σ^*, defined via (1.1) in terms of the solutions of the field equation (2.2) for $\mathbf{j}$ as a function of the applied field $\mathbf{e}$. Thus the weight matrices and normalization matrix, which are collectively denoted as fundamental geometric parameters, characterize the orientation of the n subspaces $\mathscr{P}_a$, $a = 1, 2, \ldots, n$ with respect to the three subspaces $\mathscr{U}$, $\mathscr{E}$, and $\mathscr{J}$. We label the submatrices that occur along the block diagonals of W_a and N by a superscript j, which should not be confused with the reference medium superscript q. Like any submatrix $A^{(j)}$ of a matrix $A_{\lambda,\eta}$ these submatrices $W_a^{(j)}$, $j \geq 0$, and $N^{(j)}$, $j \geq 1$, are comprised of elements $W_{a,\lambda,\eta}^{(q)}$ and $N_{\lambda,\eta}^{(q)}$ with $o(\lambda) = o(\eta) = j$, and hence each has dimension $d(n-1)^j$ which represents the number of fields $\mathbf{P}_{a\lambda}'^{(q)}$ or $\mathbf{E}_\lambda'^{(q)}$ of order j.

For an n-component composite material with isotropic components the elementary weight matrices $W_a^{(0)}$ satisfy

$$W_a^{(0)} = f_a I^{(0)}, \tag{2.11}$$

where f_a is the volume fraction of component a while the elementary normalization matrix $N^{(1)}$ has the property that

$$\text{Tr}\,[I^{(1)}+N^{(1)}]^{-1}=I,\tag{2.12}$$

where the trace extends over the direction indices but *not* over the component indices [12, 13, 1]. More generally the normalization factors $N^{(j)}$ and weight matrices $W_a^{(j)}$ are determined by the $(2j)$-point and $(2j+1)$-point correlation functions characterizing the composite geometry [42, 44, 7].

Now, following the notation adopted in Part I, we let

$$\tilde{A}=A^{-1},\quad \hat{A}=A^{1/2},\quad \dot{A}=A^{-1/2}\tag{2.13}$$

denote the inverse, square root and inverse square root of any matrix A, and given any component index $a=1,2,\ldots,n$, we let A_a with transpose A_a^T, denote the submatrix of A with elements $A_{a\tau,\,\lambda}$ labelled by the strings τ and λ. It is also convenient to define the conductivity differences

$$\delta\sigma_a\equiv\sigma_a-\sigma_q,\quad \delta\tilde\sigma_a\equiv 1/\sigma_a-1/\sigma_q,\tag{2.14}$$

for $a=1,2,\ldots,n$, and the matrix

$$Y_{a\lambda,\,b\eta}^{(q)}=\delta_{ab}W_{a,\,\lambda,\,\eta}^{(q)}-W_{a,\,\lambda,\,\tau}^{(q)}W_{b,\,\tau,\,\eta}^{(q)},\tag{2.15}$$

in which summation over τ, like any other repeated Greeks or script (but not italic) subscript, is implied.

The continued fraction expansions developed in Part I, for the effective tensor

$$\sigma^*=\Omega^{(0)}\tag{2.16}$$

are generated by eliminating the matrices $\Omega^{(j)}$ for $j\geq 1$ from the recursion relation

$$\Omega^{(j-1)}=\sum_{a=1}^{n}\sigma_a W_a^{(j-1)}-\sum_{a,\,b\neq q}\delta\sigma_a\hat{Y}_a^{(j)}$$
$$\times\left[\sigma_q I^{(j)}+\sum_{c\neq q}\delta\sigma_c\hat{Y}_c^{(j)T}\tilde{W}_c^{(j-1)}\hat{Y}_c^{(j)}+\hat{N}^{(j)}\Omega^{(j)}\hat{N}^{(j)}\right]^{-1}\hat{Y}_b^{(j)T}\delta\sigma_b,\tag{2.17}$$

or from either of its two equivalent forms

$$\Omega^{(j-1)}=\sum_{a=1}^{n}\sigma_a W_a^{(j-1)}-\sum_{a,\,b\neq q}\delta\sigma_a I_a^{(j)}$$
$$\times\left[\sigma_q\tilde{Y}^{(j)}+\sum_{c\neq q}\delta\sigma_c I_c^{(j)T}\tilde{W}_c^{(j-1)}I_c^{(j)}+\dot{Y}^{(j)}\hat{N}^{(j)}\Omega^{(j)}\hat{N}^{(j)}\dot{Y}^{(j)}\right]^{-1}I_b^{(j)T}\delta\sigma_b,\tag{2.18}$$

$$\tilde\Omega^{(j-1)}=\sum_{a=1}^{n}W_a^{(j-1)}/\sigma_a-\sum_{a,\,b\neq q}\delta\tilde\sigma_a\hat{Y}_a^{(j)}$$
$$\times\left[I^{(j)}/\sigma_q+\sum_{c\neq q}\delta\tilde\sigma_c\hat{Y}_c^{(j)T}\tilde{W}_c^{(j-1)}\hat{Y}_c^{(j)}+\dot{N}^{(j)}\tilde\Omega^{(j)}\dot{N}^{(j)}\right]^{-1}\hat{Y}_b^{(j)T}\delta\tilde\sigma_b,\tag{2.19}$$

or by eliminating $\Omega^{(j)}$ and the matrices

$$\Delta_{a,\,b}^{+\,(j)}\equiv\dot{W}_a^{(j-1)}\hat{Y}_a^{(j)}\tilde{\Pi}^{+\,(y)}\hat{Y}_b^{(j)T}\dot{W}_b^{(j-1)}-s_a I_{a,\,b}^{(j)},\tag{2.20}$$

where

$$\Pi^{+(j)} \equiv I^{(j)} + \hat{N}^{(j)} \Omega^{(j)} \hat{N}^{(j)}/\sigma_q, \tag{2.21}$$

$$s_a = s_a^{(q)} \equiv \sigma_q/(\sigma_q - \sigma_a), \tag{2.22}$$

from the relations

$$\Omega^{(j-1)}/\sigma_q = I^{(j-1)} + \sum_{a,b \neq q} \hat{W}_a^{(j-1)} \tilde{\Delta}_{a,b}^{+(j)} \hat{W}_b^{(j-1)}, \tag{2.23}$$

for all $j \geq 1$. These formulae were derived first from standard variational principles and subsequently from a new field equation recursion method. In the field equation recursion method, $\Omega^{(j)}$ is interpreted as the effective tensor associated with a field equation of the form (2.2) in the Hilbert space

$$\mathcal{H}^{(j)} = \mathcal{U}^{(j)} \oplus \mathcal{E}^{(j)} \oplus \mathcal{J}^{(j)} = \mathcal{P}_1^{(j)} \oplus \mathcal{P}_2^{(j)} \oplus \ldots \oplus \mathcal{P}_n^{(j)}, \tag{2.24}$$

where $\mathcal{U}^{(j)}$ is the $d(n-1)^j$-dimensional subspace spanned by the fields $\mathbf{x}_\omega^{(q)}$ with $o(\omega) = j$, while $\mathcal{E}^{(j)}$, $\mathcal{J}^{(j)}$, and $\mathcal{P}_a^{(j)}$ are spanned respectively by the fields $\mathbf{E}_\tau^{\prime(q)}$, $\mathbf{J}_\tau^{\prime(q)}$, and $\mathbf{P}_{a\lambda}^{\prime(q)}$ with $o(\tau) \geq j+1$ and $o(\lambda) \geq j$. Thus when $j = 0$, $\Omega^{(j)}$ can be identified with σ^* in accordance with (2.16). For $j > 0$ the solutions of the jth-order field equation generate the solutions of the $(j-1)$th-order field equation and imply the above relations between $\Omega^{(j-1)}$ and $\Omega^{(j)}$.

The variational approach yields bounds on σ^* that apply when the component conductivities σ_a, $a = 1, 2, \ldots, n$, are real or at least share the same argument in the complex plane. In I we found the $(2h+1)$th-order Wiener-Beran upper and lower bounds on σ^* are expressible as a continued fraction of the form implied by (2.17) or (2.19), but which is terminated at the hth-level by the tensor

$$\Omega^{(h)} = \sum_{a=1}^{n} \sigma_a W_a^{(h)}, \tag{2.25}$$

giving the upper bound $\sigma^* \leq \Omega^{(0)}$, or by the tensor

$$\Omega^{(h)} = \left[\sum_{a=1}^{n} W_a^{(h)}/\sigma_a \right]^{-1}, \tag{2.26}$$

giving the lower bound $\sigma^* \geq \Omega^{(0)}$. Similarly the $(2h)$th-order Hashin-Shtrikman bounds are expressible as a continued fraction of the form implied by (2.20–23) that is terminated by the tensor

$$\Omega^{(h)} = \sigma_m I^{(h)}, \tag{2.27}$$

where σ_m is chosen as either the smallest or largest component conductivity, giving respectively lower and upper bounds, $\sigma^* \geq \Omega^{(0)}$ and $\sigma^* \leq \Omega^{(0)}$. The assumed convergence of these bounds to σ^* as $h \to \infty$ (proved here in Sect. 8) implies the continued fraction expansion for σ^*.

Some sets of geometric parameters, denoted as terminating sets, correspond to Hilbert spaces $\mathcal{H}$ of finite dimension and result in a continued fraction for σ^* that terminates at some level. In I we found that the Wiener-Beran bounds and Hashin-Shtrikman bounds correspond to particular sets of terminating geometric parameters and thus represent the effective tensor σ^* in a finite dimensional

Hilbert space. The $(2h+1)$th-order Wiener-Beran upper and lower bounds are obtained by replacing the normalization factor $N^{(h+1)}$ by the terminating ones,

$$N^{(h+1)} = \infty I^{(h+1)} \quad \text{and} \quad N^{(h+1)} = 0, \tag{2.28}$$

while the $(2h)$th-order Hashin-Shtrikman bounds are obtained by replacing the weights $W_a^{(h)}$ with the terminating set

$$\begin{aligned} W_a^{(h)} &= I^{(h)} \quad \text{for} \quad a = m \\ &= 0 \quad \text{for} \quad a \neq m. \end{aligned} \tag{2.29}$$

3. Ω-Functions: Analytic and Invariance Properties

Let us consider the class of all matrix-valued functions $\sigma_{\ell k}^*(\sigma_1, \sigma_2, ..., \sigma_n)$, $\ell, k = 1, 2, ..., d$, that are expressible as a continued fraction of the form implied by (2.16) and (2.17), for some choice of positive semidefinite normalization factors and weights. Such sets of fundamental geometric parameters are called *allowable* and the functions are denoted as *n-variable Ω-functions of rank d*. The functions share many of the beautiful analytic properties characterizing the conductivity functions of real composite materials: see Bergman [16, 19], Milton [20], Dell'Antonio et al. [2], and Golden and Papanicolaou [18] for a discussion of the analytic properties pertaining to real materials. According to this definition of Ω-functions, the conductivity matrices $\Omega^{(j)}(\sigma_1, \sigma_2, ..., \sigma_n)$ for all $j \geq 0$ are clearly *n*-variable Ω-functions of rank $k \equiv dn'^j$ where $n' = n - 1$.

Some properties of Ω-functions are immediately apparent: they are *homogeneous* in the sense that

$$\sigma^*(\lambda\sigma_1, \lambda\sigma_2, ..., \lambda\sigma_n) = \lambda\sigma^*(\sigma_1, \sigma_2, ..., \sigma_n), \tag{3.1}$$

for all constants λ, and satisfy the *normalization*

$$\sigma^*(1, 1, 1, ..., 1) = I. \tag{3.2}$$

Furthermore, *the matrix inverse of an Ω-function of the variables σ_a, $a = 1, 2, ..., n$, is an Ω-function of the reciprocal variables $1/\sigma_a$* by virtue of the equivalence of (2.17) and (2.19). (In our Hilbert space this reciprocal transformation corresponds to interchanging the roles of the subspaces $\mathcal{E}$ and $\mathcal{J}$, replacing the normalization matrices $N^{(j)}$ by their reciprocals $\tilde{N}^{(j)}$, and leaving the weights unchanged.)

Additional analytic properties of Ω-functions can be established by induction. We start by proving that

$$\sigma^* > 0 \quad \text{when} \quad \sigma_a > 0 \quad \forall a. \tag{3.3}$$

To do this, choose the reference variable σ_q as the minimum of all the σ_a, $a = 1, 2, ..., n$, to ensure the inequality

$$s_a^{(q)} \leq 0 \tag{3.4}$$

is satisfied for all a. Now consider those terminating continued fractions for which $\Omega^{(h)}$ is given by (2.26): this effective tensor, $\Omega^{(h)}$, is clearly strictly positive definite. So suppose $\Omega^{(j)} > 0$ for some $j \leq h$. This implies, via (2.20) and (2.21) that

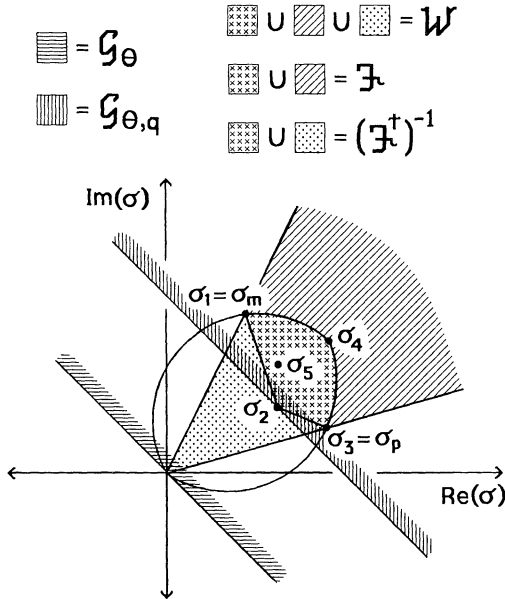$$\Pi^{+(j)} \geq 0, \quad \Delta^{+(j)} \geq 0, \tag{3.5}$$

Fig. 1. Sketch illustrating the various regions in the complex plane that are needed to construct the bounds of Sect. 4 for a five component composite with complex component conductivities $\sigma_1, \sigma_2, ..., \sigma_5$. The half-planes $\mathscr{G}_\theta$ and $\mathscr{G}_{\theta,q}$, shown here with $\theta = -\pi/4$ and $q=2$, are shaded only along their boundaries. The wedge $\mathscr{W}$ extends out to infinity

when the variables $s_a^{(q)}$ are all negative as in (3.4). Consequently, from (2.23) we deduce that $\Omega^{(j-1)} > 0$ and by induction it follows that $\Omega^{(0)} > 0$ for all terminating continued fractions of the type we considered. The convergence from below of $\Omega^{(0)}$ to σ^* in the limit $h \to \infty$ (as established in Sect. 8) subsequently implies that $\sigma^* > 0$.

Next we demonstrate that for complex-valued variables,

$$\text{Im}\,\sigma^* > 0 \quad \text{when} \quad \text{Im}\,\sigma_a > 0 \quad \forall a. \tag{3.6}$$

The reference variable $\sigma_q (= \sigma_a$ for some a) is chosen so the line joining σ_q to the origin does not pass through the convex hull of the n points σ_a, $a = 1, 2, ..., n$. Then there exists some angle θ such that all the points σ_a, $a = 1, 2, ..., n$, but not the origin are contained in the half plane, $\mathscr{G}_{\theta,q}$, that has its boundary passing through σ_q at an angle θ: see Fig. 1. This ensures

$$\text{Im}(e^{-i\xi} s_a^{(q)}) \geqq 0 \quad \forall a, \quad \text{where} \quad \xi \equiv (\arg \sigma_q - \theta). \tag{3.7}$$

To prove (3.6) by induction consider the class of terminating continued fractions for which $\Omega^{(h)}$ is given by (2.25), (2.26) or (2.27) and assume

$$\text{Im}(e^{-i\theta} \hat{N}^{(j)} \Omega^{(j)} \hat{N}^{(j)}) \geqq 0, \tag{3.8}$$

or equivalently that

$$\text{Im}(e^{i\xi} \hat{N}^{(j)} \Omega^{(j)} \hat{N}^{(j)} / \sigma_q) \geqq 0, \tag{3.9}$$

for some $j \leqq h$: this is certainly true when $j = h$, as ensured by (3.7).

Now for any symmetric matrix A, we have $\text{Im} A \geqq 0$ if and only if the inequality

$$\text{Im}(\bar{\tau}^T A \tau) \geqq 0 \tag{3.10}$$

holds for all complex vectors τ, where $\bar{\tau}^T$ denotes the complex conjugate of the transpose of τ. By substituting $\tau = A^{-1}\eta$, where η is any complex vector we deduce

$$\text{Im} A \geqq 0 \quad \text{iff} \quad \text{Im} A^{-1} \leqq 0. \tag{3.11}$$

It immediately follows from this, (3.8) and (2.21) that

$$\text{Im}[e^{-i\xi}(\Pi^{+(j)})^{-1}] \leqq 0, \tag{3.12}$$

which in conjunction with (2.20) and (3.7) implies

$$\text{Im}(e^{-i\xi}\Delta^{+(j)}) \leqq 0. \tag{3.13}$$

This in turn leads through (2.23) to the bound

$$\text{Im}[e^{-i\theta}(\Omega^{(j-1)} - \sigma_q I^{(j-1)})] \geqq 0, \tag{3.14}$$

which implies (3.8) is satisfied when j is replaced by $j-1$. Note further that (3.14) holds when $j-1=h$. Thus both inequalities (3.14) and (3.8) are established. In particular, if the variables σ_a all have non-negative imaginary parts and σ_q is chosen so $\text{Im}\,\sigma_q \leqq \text{Im}\,\sigma_a$ for all a, then we can take $\theta = 0, j = 1$ and our result (3.14) implies

$$\text{Im}\,\Omega^{(0)} > 0 \quad \text{when} \quad \text{Im}\,\sigma_a > 0 \quad \forall a. \tag{3.15}$$

Taking the limit $h \to \infty$, establishes (3.6). The tighter inequality (3.14) will be needed for deriving bounds in Sect. 4: it implies for all real unit vectors α that $\alpha^T \Omega^{(j)} \alpha$ is inside the half-plane $\mathscr{G}_{\theta,q}$ containing the points σ_a, $a = 1, 2, ..., n$.

In Sect. 8 of Part I we proved that there is always a Hilbert space

$$\mathscr{H} = \mathscr{U} \oplus \mathscr{E} \oplus \mathscr{J} = \mathscr{P}_1 \oplus \mathscr{P}_2 \oplus ... \oplus \mathscr{P}_n \tag{3.16}$$

associated with any set of positive-semidefinite fundamental geometric parameters. The allowable geometric parameters can be chosen as the set that occur in the continued fraction expansion of an Ω-function, and the Ω-function then represents the effective tensor in $\mathscr{H}$. This *Hilbert space correspondence* is a powerful tool for establishing properties of Ω-functions. Indeed, the Thompson variational principle, (12.23) in I, directly implies (3.3) and similarly (3.6) follows from elementary considerations in the Hilbert space $\mathscr{H}$ [53, 55].

Now since we are free to choose our reference variable σ_q as any of the σ_a, $a = 1, 2, ..., n$, an Ω-function will remain an Ω-function *under any interchange of variables*. Also, because it doesn't matter what set of orthonormal vectors $\mathbf{x}_\ell$, $\ell = 1, 2, ..., d$, are chosen to span $\mathscr{U}$, an Ω-function will remain an Ω-function *under orthogonal transformations*.

Alternatively we can select any subset of the basis vectors $\mathbf{x}_\ell$, say those vectors with $\ell \leqq d^\vee$, that span a subspace $\mathscr{U}^\vee \subset \mathscr{U}$ of dimension $d^\vee < d$. The remaining vectors $\mathbf{x}_\ell$ with $\ell > d^\vee$ span a subspace $\bar{\mathscr{U}}^\vee$ which is the $(d - d^\vee)$-dimensional orthogonal complement of $\mathscr{U}^\vee$ in $\mathscr{U}$. Our Hilbert space $\mathscr{H}$ is clearly spanned by the three mutually orthogonal subspaces

$$\mathscr{U}^\vee, \mathscr{E}^\vee \equiv \mathscr{E}, \mathscr{J}^\vee \equiv \mathscr{J} \oplus \bar{\mathscr{U}}^\vee, \tag{3.17}$$

and in this Hilbert space the field equation (2.2) has solutions for $\mathbf{j} \in \mathscr{U}$, $\mathbf{J}^* \in \mathscr{J}$, and $\mathbf{E}^* \in \mathscr{E}^{\vee}$ given any $\mathbf{e} \in \mathscr{U}^{\vee}$. Note the current field $\mathbf{j} + \mathbf{J}^*$ can be re-expressed as $\mathbf{j}^{\vee} + \mathbf{J}^{*\vee}$, where

$$\mathbf{j}^{\vee} \equiv \Gamma_0^{\vee} \mathbf{j} \in \mathscr{U}^{\vee}, \qquad \mathbf{J}^{*\vee} \equiv \mathbf{J}^* + (I - \Gamma_0^{\vee}) \mathbf{j} \in \mathscr{J}^{\vee}, \tag{3.18}$$

in which $\Gamma_0^{\vee}$ is the projection operator onto $\mathscr{U}^{\vee}$. Consequently if $\sigma_{\ell k}^*$, $\ell, k \leq d$, is an Ω-function of rank d, then the truncated matrix $\sigma_{\ell k}^*$, $\ell, k \leq d^{\vee}$ is an Ω-function of rank $d^{\vee}$ for all $d^{\vee} \leq d$. Thus an Ω-function remains an Ω-function *after matrix truncation*. In particular, the d diagonal elements of an Ω-function of rank d must be scalar Ω-functions.

From the Hilbert space correspondence it is clear that an Ω-function remains an Ω-function under *contraction of variables*. That is, for any $a, b \in \{1, 2, ..., n\}$ with $a \neq b$ we are free to set $\sigma_a = \sigma_b$ in an n-variable Ω-function to produce an $(n-1)$-variable Ω-function. In our Hilbert space this is equivalent to replacing $\mathscr{P}_a$ and $\mathscr{P}_b$ by $\mathscr{P}_a \oplus \mathscr{P}_b$, thereby reducing the number of subspaces $\mathscr{P}_a$ from n to $n-1$.

The class of Ω-functions also satisfy an important convexity property, which follows from the Hilbert space correspondence. In Appendix 1 it is established that the weighted arithmetic (or harmonic) mean of two n-variable Ω-functions of the same rank, d, is an n-variable Ω-function of rank d. Thus *the average of a set of Ω-functions is an Ω-function*.

Another way of generating a new Ω-function $^\dagger\sigma^*(\sigma_1, \sigma_2, ..., \sigma_n)$ from a given Ω-function $\sigma^*(\sigma_1, \sigma_2, ..., \sigma_n)$ is to choose any fixed positive real scaling factor $\lambda < \infty$, introduce the normalization matrix,

$$^\dagger N = \sigma^*(\lambda, 1, 1, 1, ..., 1), \tag{3.19}$$

and take

$$^\dagger\sigma^*(\sigma_1, \sigma_2, \sigma_3, ..., \sigma_n) \equiv {}^\dagger\dot{N}\sigma^*(\lambda\sigma_1, \sigma_2, \sigma_3, ..., \sigma_n)^\dagger\dot{N}. \tag{3.20}$$

The invariance of the class of Ω-functions under this *renormalized single variable rescaling* defined by (3.20) is rigorously proved in Appendix 2, for all real $\lambda > 0$. Physically, in any n-component impedance network and for any integer $\lambda > 0$, this rescaling corresponds to replacing each impedance of component 1 by λ impedances of component 1 connected in parallel: the Ω-function $^\dagger\sigma^*(\sigma_1, \sigma_2, ..., \sigma_n)$ given by (3.20) represents the response of the resulting network.

Clearly the isotropic component materials in a heterogeneous medium can themselves be taken as composites, provided their microstructure is much smaller than the inhomogeneities in the heterogeneous medium in which they are embedded. This suggests that any one of the variables, say $'\sigma_1$, in an n-variable tensor Ω-function $'\sigma^*('\sigma_1, '\sigma_2, ..., '\sigma_n)$ can be replaced by an m-variable scalar Ω-function $''\sigma^*(''\sigma_1, ''\sigma_2, ..., ''\sigma_m)$ to produce an $(n+m-1)$-variable Ω-function,

$$\sigma^*(\sigma_1, \sigma_2, ..., \sigma_{n+m-1}) \equiv '\sigma^*(''\sigma^*(\sigma_1, \sigma_2, ..., \sigma_m), \sigma_{m+1}, \sigma_{m+2}, ..., \sigma_{n+m-1}). \tag{3.21}$$

The proof that a *scalar Ω-function can indeed be substituted in a given rank d Ω-function to produce a new rank d Ω-function* is given in Appendix 3.

Let us define a *Σ-function* as any n-variable, symmetric matrix-valued function $\sigma^*(\sigma_1, \sigma_2, ..., \sigma_n)$ satisfying (3.1), (3.3), and (3.6). The class of *normalized Σ-functions*, that in addition satisfy the normalization (3.2) is the class which has been

extensively studied by Bergman [16, 19], Milton [20], and most recently by Dell'Antonio et al. [2] and Golden and Papanicolaou [18], usually with $d = 1$. We have established that any Ω-function is a normalized Σ-function and it is tempting to conjecture that the converse is also true. Indeed, normalized Σ-functions satisfy *all* those properties of Ω-functions established above, and there is currently no evidence to suggest a distinction between the two classes of analytic function.

The continued fraction expansion for normalized *two-variable* Σ-functions derived in Appendix 4 confirms their equivalence with Ω-functions when $n = 2$. Successive normalization factors and weights are uniquely determined by matching terms in the series expansion for σ^* in powers of $\delta\sigma \equiv \sigma_1 - \sigma_2$. Unfortunately such a simple algorithm does not extend to multivariate functions, with $n \geq 3$. Indeed the coefficients in the series expansion for σ^*, up to third-order (or any higher *finite* order) in the differences $\delta\sigma_a^{(q)} = \sigma_a - \sigma_q$, incorporate more unknown geometric parameters than there are coefficients to solve for them. Thus, in a three variable Ω-function (with $n = 3$) the number of independent geometric parameters in the normalization factor $N^{(j)}$ (or in the set of weights $W_a^{(j)}$, $a = 1, 2, ..., n$) increases exponentially with j, as 2^{j-1} (or 2^j) for large j, whereas the number of independent coefficients of order $2j$ (or $2j + 1$) in the series expansion for σ^* increases only linearly with j, as $2j + 1$ (or $2j + 2$). Consequently, there cannot be any direct relation between truncated continued fractions (which incorporate the weights and normalization factors) and multivariate rational approximants, such as the Canterbury approximants [51] (which incorporate the series expansion coefficients).

This raises the basic question: are the normalization factors and weights uniquely determined by the analytic behavior of σ^* as a function of the variables σ_a, $a = 1, 2, ..., n$? While there is a mismatch between the number of geometric parameters, in the normalization factors and weight matrices, and the coefficients in the series expansion at any finite order, this does not exclude the possibility that the countably infinite set of series coefficients suffices to determine the countably infinite set of geometric parameters. (Of course we should disregard the trivial degeneracies associated with terminating sets of geometric parameters, namely that the higher-order weights and normalization factors do not influence σ^*.) For composites the issue is not of fundamental importance because the geometric parameters can (in principle) be determined directly from the correlation functions and there is no need to analyze series expansions for σ^*. However, the question clearly deserves attention if the continued fraction expansion are to be related to the Golden-Papanicolaou integral representations for the function $\sigma^*(\sigma_1, \sigma_2, ..., \sigma_n)$ [53, 55]. And of course it would be interesting to know the analytic significance of the weight matrices and normalization factors.

4. Hierarchies of Bounds on Ω-Functions

In practice the m-point correlation functions characterizing the geometry of a composite will be known up to some odd order $2g - 1$ (or even order $2g$) that is typically small. From these correlation functions we can in principle calculate the weights $W_a^{(j)}$ and the normalization factors $N^{(j)}$ (or $N^{(j+1)}$) for all $j \leq g - 1$. Our

objective here is to bound σ^* given these fundamental geometric parameters and the (real or complex) component conductivities σ_a, $a = 1, 2, ..., n$. This is accomplished by treating the more general problem of bounding Ω-functions.

Suppose the weights $W_a^{(j)}$ and the normalization factors $N^{(j)}$ are known for all $j \leq g - 1$, and let us assume all the variables σ_a all lie in one half of the complex plane. Define $\mathscr{W}$ as the *smallest wedge* in the complex plane with sides meeting at the origin that contains all the points σ_a, $a = 1, 2, ..., n$, and let σ_m and σ_p label two variables in the set $\{\sigma_1, \sigma_2, ..., \sigma_n\}$ that lie on opposite sides of the wedge $\mathscr{W}$, with $\arg \sigma_m \geq \arg \sigma_p$. Also for any angle θ in the range

$$\arg \sigma_p \geq \theta \geq -\pi + \arg \sigma_m, \tag{4.1}$$

let $\mathscr{G}_\theta$ denote the *half-plane*, containing $\mathscr{W}$, that has boundary passing through the origin at an angle θ to the real axis: see Fig. 1.

From the special properties (3.1) and (3.6) of Ω-functions, such as $\Omega^{(g)}(\sigma_1, \sigma_2, ..., \sigma_n)$, any half-plane passing through the origin and containing all the points σ_a, $a = 1, 2, ..., n$, must necessarily contain $\alpha^T \Omega^{(g)} \alpha$ for all real vectors α. Hence by defining

$$\Lambda^{(g)} \equiv \sigma_q(\Pi^{+(g)} - I^{(g)}) = \hat{N}^{(g)} \Omega^{(g)} \hat{N}^{(g)}, \tag{4.2}$$

we have *the elementary half-plane bounds on* $\Lambda^{(g)}$,

$$\alpha^T \Lambda^{(g)} \alpha \in \mathscr{G}_\theta \quad \text{for all real } \alpha. \tag{4.3}$$

Now given any integer $k > 0$ and region $\mathscr{R}$ of the complex plane, let us define $\mathscr{S}(k, \mathscr{R})$ as the set of symmetric, complex $k \times k$ matrices A, such that

$$A \in \mathscr{S}k, \mathscr{R}) \quad \text{iff} \quad \alpha^T A \alpha / (\alpha^T \alpha) \in \mathscr{R} \quad \text{for all real } \alpha \neq 0. \tag{4.4}$$

With this simplified notation the elementary half-plane bounds (4.3) take the form

$$\Lambda^{(g)} \in \mathscr{S}(dn'^g, \mathscr{G}_\theta), \tag{4.5}$$

where $n' \equiv n - 1$. Since $\mathscr{W}$ is the region of intersection of all the half-planes $\mathscr{G}_\theta$, with θ between the limits (4.1), $\Lambda^{(g)}$ must satisfy *the elementary wedge bounds*

$$\Lambda^{(g)} \in \mathscr{S}(dn'^g, \mathscr{W}). \tag{4.6}$$

Remarkably, the converse is also true: for any given matrix Λ in $\mathscr{S}(dn'^g, \mathscr{W})$ there exists an allowable set of geometric parameters such that

$$\Lambda^{(g)} = \Lambda. \tag{4.7}$$

To see this, we will first suppose the variables σ_m and σ_p, which lie on opposite sides of the wedge $\mathscr{W}$, satisfy $\arg \sigma_m \neq \arg \sigma_p$. Then for any complex matrix $\Lambda \in \mathscr{S}(dn'^g, \mathscr{W})$ there exist real symmetric matrices

$$\Lambda_m = [\text{Im}(\sigma_m/\sigma_p)]^{-1} \text{Im}(\Lambda/\sigma_p) \geq 0,$$
$$\Lambda_p = [\text{Im}(\sigma_p/\sigma_m)]^{-1} \text{Im}(\Lambda/\sigma_m) \geq 0, \tag{4.8}$$

such that Λ can be represented in the form

$$\Lambda = \sigma_m \Lambda_m + \sigma_p \overline{\Lambda_p} \quad \text{with} \quad \Lambda_m \geq 0, \quad \Lambda_p \geq 0. \tag{4.9}$$

In the special case where $\arg\sigma_m=\arg\sigma_p$, the wedge $\mathscr{W}$ degenerates into a single ray extending from the origin and obviously Λ can still be expressed in the form (4.9) with $\Lambda_p=0$ and $\Lambda_m\geqq0$. In either circumstance we choose the terminating set of allowable geometric parameters

$$N^{(g)}=\Lambda_m+\Lambda_p, \qquad N^{(g+1)}=\infty I^{(g+1)},$$
$$W_a^{(g)}=\dot{N}^{(g)}\Lambda_a\dot{N}^{(g)} \quad \text{for} \quad a=m \quad \text{or} \quad p$$
$$=0 \qquad\qquad\qquad \text{otherwise}, \tag{4.10}$$

which results in a conductivity matrix $\Omega^{(g)}$ given exactly by (2.25), with h replaced by g. Hence we have

$$\hat{N}^{(g)}\Omega^{(g)}\hat{N}^{(g)}=\Lambda, \tag{4.11}$$

and with (4.2) this implies that (4.7) is indeed satisfied for the above choice of geometric parameters. *Therefore the elementary wedge bounds* (4.5) *form the most restrictive bounds that can be placed on* $\Lambda^{(g)}$, *and hence* $\Pi^{+(g)}$ *without further knowledge about the geometric parameters.*

Now σ^* depends on $\Pi^{+(g)}$, and hence $\Lambda^{(g)}$ through (2.16) and the recursion relations (2.20–23) which thus define a function $\sigma_g^*(\Lambda^{(g)})$ giving

$$\sigma^*=\sigma_g^*(\Lambda^{(g)})=\sigma_g^*(\Lambda^{(g)};\sigma_a,W_a^{(j)},N^{(j)}) \tag{4.12}$$

in terms of $\Lambda^{(g)}$, the conductivity variables σ_a and the known geometric parameters $W_a^{(j)}$ and $N^{(j)}$ with $j\geqq g-1$. This function $\sigma_g^*(\Lambda^{(g)})$ can be regarded as a mapping from the set of symmetric complex dn'^g-dimensional matrices to the set of symmetric complex d-dimensional matrices. From (4.5) and (4.12) we have the $(2g-1)$*th-order half-plane bounds,*

$$\sigma^*\in\sigma_g^*(\mathscr{S}(dn'^g,\mathscr{G}_\theta)), \tag{4.13}$$

while (4.6) implies the $(2g-1)$*th-order wedge bounds,*

$$\sigma^*\in\sigma_g^*(\mathscr{S}(dn'^g,\mathscr{W})). \tag{4.14}$$

Since the elementary wedge bounds are optimal, these wedge bounds (4.14) are the best-possible bounds on n-variable Ω-functions of rank d, given $W_a^{(j)}$, $a=1,2,...,n$, and $N^{(j)}$ for all $j\geqq g-1$ and no other information about the successive geometric parameters.

When the variables σ_a are all real, (4.6) implies the optimal bounds,

$$I^{(g)}\leqq\Pi^{+(g)}\leqq\infty I^{(g)}, \tag{4.15}$$

which together with (2.20) and (2.23) yields (at some loss of information on correlations between eigenvalues) the bounds

$$\left(\sum_{a=1}^n W_a^{(g-1)}/\sigma_a\right)^{-1}\leqq\Omega^{(g-1)}\leqq\sum_{a=1}^n W_a^{(g-1)}\sigma_a. \tag{4.16}$$

Thus the Wiener-Beran bounds of order $2g-1$ follow from the wedge bounds, (4.14). In fact *the wedge bounds are generally tighter than the Wiener-Beran bounds when* $d>1$ *and* $g>1$ because they incorporate additional restrictions on the correlations between the different eigenvalues of σ^*. Although the Wiener-Beran

bounds are individually attainable [as the effective tensor in a Hilbert space of the form (2.9) characterized by a set of geometric parameters terminated by (2.28)] it is incorrect to infer the attainability of every conductivity matrix between these bounds: such a matrix may have some eigenvalues coinciding with the upper bound and other eigenvalues coinciding with the lower bound. For scalar Ω-functions the attainability of the Wiener-Beran bounds (and the Hashin-Shtrikman bounds) of course implies their optimality to all orders.

If in addition the normalization factor $N^{(g)}$ is known then the wedge bounds can be improved. The half-plane $\mathscr{G}_{\theta,q}$, as defined in Sect. 3 and illustrated in Fig. 1, is a translation of $\mathscr{G}_\theta$ by the amount σ_q. To ensure $\mathscr{G}_{\theta,q}$ contains all the variables σ_a, $a = 1, 2, ..., n$, but not the origin, we require that θ satisfy (4.1) and second that the reference variable σ_q is chosen with

$$\operatorname{Im}(e^{-i\theta}\sigma_q) \leqq \operatorname{Im}(e^{-i\theta}\sigma_a) \quad \forall a. \tag{4.17}$$

The intersection of all such planes forms an open polygon $\mathscr{F}$ (see Fig. 1) which is the convex hull of n rays that issue from the points σ_a, $a = 1, 2, ..., n$, at angles $\arg\sigma_a$. (Thus each ray when extended in the opposite direction passes through the origin.)

Since (3.14) is satisfied whenever (3.7) holds, we deduce that any half plane containing the points σ_a, $a = 1, 2, ..., n$, also contains $\boldsymbol{\alpha}^T\Omega^{(j)}\boldsymbol{\alpha}$ for all real unit vectors $\boldsymbol{\alpha}$. This implies the *elementary half-plane bounds on* $\Omega^{(g)}$,

$$\Omega^{(g)} \in \mathscr{S}(dn'^g, \mathscr{G}_{\theta,q}). \tag{4.18}$$

Others bounds are obtained by noting that $\tilde{\Omega}^{(g)}$ is an Ω-function of the variables $1/\sigma_a$. Specifically we select σ_q so that

$$\operatorname{Im}(e^{i\theta}/\sigma_q) \geqq \operatorname{Im}(e^{i\theta}/\sigma_a) \quad \forall a, \tag{4.19}$$

and define the half-plane $\mathscr{G}_{\theta,q}^\dagger$ to be a translation of the complex conjugate of $\mathscr{G}_\theta$ (i.e. the inverse of $\mathscr{G}_\theta$) through an amount $1/\sigma_q$. The intersection of all such half-planes forms an open polygon $\mathscr{F}^\dagger$ which is the convex hull of the n rays emanating from the points $1/\sigma_a$, $a = 1, 2, ..., n$, extending away from the origin at angles $\arg(1/\sigma_a)$.

By analogy with (4.18) we have the *elementary half-plane reciprocal bounds on* $\Omega^{(g)}$,

$$\Omega^{(g)} \in \tilde{\mathscr{S}}(dn'^g, \mathscr{G}_{\theta,q}^\dagger), \tag{4.20}$$

where $\tilde{\mathscr{S}}(k, \mathscr{R})$ denotes the set of matrices that have an inverse in $\mathscr{S}(k, \mathscr{R})$. Since (4.18) and (4.20) hold for all combinations of half-planes $\mathscr{G}_{\theta,q}$ and $\mathscr{G}_{\theta,q}^\dagger$ we deduce the *elementary polygon bounds on* $\Omega^{(g)}$

$$\Omega^{(g)} \in \mathscr{S}(dn'^g, \mathscr{F}) \cap \tilde{\mathscr{S}}(dn'^g, \mathscr{F}^\dagger), \tag{4.21}$$

which are better than the elementary wedge bounds (4.6) because $\mathscr{F} \subset \mathscr{W}$ and $(\mathscr{F}^\dagger)^{-1} \subset \mathscr{W}$. For scalar Ω-functions these polygon bounds imply

$$\sigma^* \in \mathscr{F} \cap (\mathscr{F}^\dagger)^{-1}, \quad \text{when} \quad d = 1, \tag{4.22}$$

which in fact coincide with the known elementary bounds [28, 54] on scalar normalized Σ-functions and are *realizable* by the diagonal elements of σ^* of real

composite materials. The straight edge (or circular arc) between any adjacent pair of vertices σ_a and σ_b of $\mathscr{F}$ [or $(\mathscr{F}^\dagger)^{-1}$] is realized by the diagonal element $\sigma_{22}^* = c\sigma_a + (1-c)\sigma_b$ (or by the diagonal element $\sigma_{11}^* = [c/\sigma_a + (1-c)/\sigma_b]^{-1}$) of the conductivity tensor of a laminate of the components σ_a and σ_b in proportions c and $(1-c)$ oriented so the direction vector $\mathbf{x}_1$ is normal to the layers. As c is varied from 1 to 0 the edge (or arc) is traced from vertex σ_a to vertex σ_b.

From the definitions (4.2) and (4.12) of $\Lambda^{(g)}$ and the function $\sigma_g^*(\Lambda^{(g)})$ the elementary bounds (4.18), (4.20), and (4.21) imply the $(2g)$ *th-order half-plane bounds*

$$\sigma^* \in \sigma_g^*(\hat{N}^{(g)}\mathscr{S}(dn'^g, \mathscr{G}_{\theta,q})\hat{N}^{(g)}), \tag{4.23}$$

the $(2g)$ *th-order half-plane reciprocal bounds*

$$\sigma^* \in \sigma_g^*(\hat{N}^{(g)}\tilde{\mathscr{S}}(dn'^g, \mathscr{G}_{\theta,q}^\dagger)\hat{N}^{(g)}), \tag{4.24}$$

and the more restrictive $(2g)$ *th-order polygon bounds*

$$\sigma^* \in \sigma_g^*(\hat{N}^{(g)}[\mathscr{S}(dn'^g, \mathscr{F}) \cap \tilde{\mathscr{S}}(dn'^g, \mathscr{F}^\dagger)]\hat{N}^{(g)}) \tag{4.25}$$

on the Ω-function σ^*.

When the variables σ_a are all real, the regions $\mathscr{F}$ and $\mathscr{F}^\dagger$ reduce to intervals on the real axis extending from σ_U and $1/\sigma_L$ to infinity, where

$$\sigma_U \equiv \max_a \sigma_a, \qquad \sigma_L \equiv \min_a \sigma_a \tag{4.26}$$

are the maximum and minimum component conductivities. In conjunction with (4.21) this implies

$$\sigma_L I^{(g)} \leqq \Omega^{(g)} \leqq \sigma_U I^{(g)}. \tag{4.27}$$

Thus the polygon bounds imply (and are generally tighter than) the Hashin-Shtrikman bounds of order $2g$. Furthermore *the polygon bounds are optimal over the class of Ω-functions, for all orders g when the variables σ_a, $a = 1, 2, ..., n$, are all real*. Thus, given any real symmetric matrix Ω satisfying the bounds (4.27) there exists an allowable conductivity matrix $\Omega^{(g)}$, such that $\Omega^{(g)} = \Omega$: for example we may take

$$\Omega^{(g)} = W_L^{(g)}\sigma_L + W_U^{(g)}\sigma_U, \tag{4.28}$$

where

$$\begin{aligned} W_L^{(g)} &= (\sigma_U I^{(g)} - \Omega)/(\sigma_U - \sigma_L) \geqq 0, \\ W_U^{(g)} &= (\Omega - \sigma_L I^{(g)})/(\sigma_U - \sigma_L) \geqq 0 \end{aligned} \tag{4.29}$$

are allowable geometric parameters.

I suspect that the polygon bounds are generally not optimal over the class of Ω-functions when the variables σ_a are complex. To obtain a complete optimal set of complex bounds of order $2g$ it may prove necessary to calculate the $(2g+1)$th-order wedge bounds and let the weights $W_a^{(g)}$ vary over all positive-semidefinite matrices satisfying (2.7). The union of the resulting sets of possible values for σ^* is guaranteed to represent the optimal $(2g)$th-order bounds on Ω-functions because the wedge bounds are optimal.

Although they are not generally optimal, the half-plane bounds have many desirable features. Their chief advantage, demonstrated in Sect. 6, is that they are

easy to calculate: in fact for scalar Ω-functions they are simply circles in the complex σ^* plane. Also, at fixed θ, the jth-order half-plane bounds, $j = 0, 1, 2, \ldots, \infty$, form a *nested sequence* of bounds, denoted as a θ-*sequence of half-plane bounds*. Thus, the $(2g)$th-order half-plane bounds are more restrictive than the $(2g-1)$th-order half-plane bounds which in turn are more restrictive than the $(2g-2)$th-order half-plane bounds: this is established by noting $\mathscr{G}_{\theta, q} \subset \mathscr{G}_\theta$ and that (3.14) is implied by (3.8). Furthermore, the property (3.11) of matrices implies the odd-order half-plane reciprocal bounds are the same as the odd-order half-plane bounds. In conjunction with the even-order half-plane reciprocal bounds they form a nested θ-*sequence of half-plane reciprocal bounds*. When θ reaches its extreme values of $\arg \sigma_p$ and $-\pi + \arg \sigma_m$ the three half-planes $\mathscr{G}_\theta$, $\mathscr{G}_{\theta, q}$ and $(\mathscr{G}_{\theta, q}^\dagger)^{-1}$ coalesce, and hence the even-order half-plane and half-plane reciprocal bounds merge with the preceding odd-order half-plane bounds.

As θ is varied between the limits (4.1) σ^* must clearly lie within the intersection of all the resulting jth-order half-plane and half-plane reciprocal bounds. This intersection defines the *inner hull* of the jth-order half-plane bounds. The nesting of the half-plane and half-plane reciprocal bounds implies that the inner hulls of these bounds, for $j = 0, 1, \ldots, \infty$, form a nested sequence of bounds.

When the variables σ_a, $a = 1, 2, \ldots, n$, are all real and positive the half-plane bounds for $\theta = -\varepsilon$ and $\theta = -\pi + \varepsilon$ (where ε is infinitesimal) imply that the inner hull only consists of real matrices σ^*. Further elementary analysis, with $\theta = -\pi/2$, establishes that the inner hull of the jth-order half-plane bounds, for $j = 1, 2, \ldots, \infty$, is at least as restrictive as the jth-order Wiener-Beran-Hashin-Shtrikman bounds.

Bounds that are narrower than the wedge or polygon bounds, yet which incorporate the same set of geometric parameters, are obtainable from additional constraints on the normalization factors and weights. These constraints are only appropriate to select classes of problems, such as conduction in composites with isotropic components, and the resulting bounds correspondingly have limited applications. As an example consider any 2-component, 2-dimensional anisotropic composite with real component conductivities labelled so that $\sigma_1 \geqq \sigma_2$. In I it was established that the associated normalization matrices $N^{(g)}$, $g = 1, 2, 3, \ldots$, have unit determinant. Hence they satisfy

$$\mathrm{Tr}[I^{(g)} + N^{(g)}]^{-1} = 1. \tag{4.30}$$

Combining this with the elementary polygon bounds (3.27) and the definition (2.21) of $\Pi^{+(g)}$ gives one of two *elementary trace bounds*,

$$\mathrm{Tr}(\tilde{\Pi}^{+(g)}) \geqq 1 \quad \text{or} \quad \mathrm{Tr}(\tilde{\Pi}^{+(g)}) \leqq 1, \tag{4.31}$$

according to whether $\sigma_q = \sigma_1$ or $\sigma_q = \sigma_2$. By expressing $\tilde{\Pi}^{+(g)}$ in terms of σ^* via the recursion relations (2.20–23) and substituting the result in (4.31) we thus obtain a hierarchy of lower and upper $(2g-1)$*th-order trace bounds* on σ^* indexed by the integer $g \geqq 1$. In particular when $g = 1$ (4.31) implies the bounds

$$\mathrm{Tr}[(\sigma^* - \sigma_2 I)^{-1}] \leqq [f_2 \sigma_1 + (1 + f_1) \sigma_2] / [f_1 \sigma_2 (\sigma_1 - \sigma_2)],$$
$$\mathrm{Tr}[(\sigma_1 I - \sigma^*)^{-1}] \leqq [f_1 \sigma_2 + (1 + f_2) \sigma_1] / [f_2 \sigma_1 (\sigma_2 - \sigma_1)], \tag{4.32}$$

which are identical to the bounds derived by Murat and Tartar [10] and by Lurie and Cherkaev [11]. In fact the above analysis closely follows the approach used by Milton and Golden to prove these bounds from the analytic properties of $\sigma^*(\sigma_1, \sigma_2)$: see [12, 27, 55]. Here we have made the generalization to include information about higher order geometric parameters. Note, however, that the hierarchy of trace bounds on σ^* implied by (4.31) supplements rather than replaces the hierarchy of wedge bounds. Unlike the wedge bounds, they are not easily extended to complex σ_1 and σ_2.

5. Representation of $\sigma_g^*(\Lambda^{(g)})$ as a Fractional Linear Matrix Transformation

The evaluation of the $(2g-1)$th-order wedge or half-plane bounds or the $(2g)$th-order polygon, half-plane or half-plane reciprocal bounds is not easy for composites with more than two components. We need to construct sets of $d \times d$ matrices that are the image, under the mapping $\sigma_g^*(\Lambda^{(g)})$, of various sets of (typically enormous) $dn'^g \times dn'^g$ complex matrices. Although this can be done numerically via repeated substitutions in the continued fraction representations for $\sigma_g^*(\Lambda^{(g)})$, it is clearly of interest to simplify this mapping.

Here we establish, by induction, that the function $\sigma_g^*(\Lambda^{(g)})$ is a *fractional linear matrix transformation* of $\Lambda^{(g)}$ expressible in the form

$$\sigma_g^*(\Lambda^{(g)}) = Q_g - R_g^T (\Lambda^{(g)} + S_g)^{-1} R_g, \tag{5.1}$$

for an appropriate choice of complex matrices Q_g, R_g, and S_g that depend not on $\Lambda^{(g)}$ but only on the variables σ_a, and the known geometric parameters $W_a^{(j)}$ and $N^{(j)}$ with $j < g$: R_g is a rectangular $dn'^g \times d$ matrix while Q_g and S_g are symmetric $d \times d$ and $dn'^g \times dn'^g$ matrices.

First note that the recursion relations (2.17) with (2.16) implies $\sigma_g^*(\Lambda^{(1)})$ can be expressed in the form (5.1) with

$$Q_1 = \sum_{a=1}^{n} \sigma_a W_a^{(0)}, \qquad R_1 = \sum_{a \neq q} \delta\sigma_a^{(q)} \hat{Y}_a^{(1)T},$$

$$S_1 = \Theta^{(1)} = \sigma_q I^{(1)} + \sum_{c \neq q} \delta\sigma_c^{(q)} \hat{Y}_c^{(1)T} \tilde{W}_c^{(0)} \hat{Y}_c^{(1)}. \tag{5.2}$$

So suppose (5.1) is satisfied for some g, say $g = j - 1$. According to the definition (4.2) of $\Lambda^{(j-1)}$, together with the recursion relation (2.18) we have

$$S_{j-1} + \Lambda^{(j-1)} = A + \sum_{a,b \neq q} B_a \tilde{C}_{a,b} B_b, \tag{5.3}$$

where

$$A = S_{j-1} + \sum_{a=1}^{n} \sigma_a \hat{N}^{(j-1)} W_a^{(j-1)} \hat{N}^{(j-1)}, \qquad B_a = \delta\sigma_a^{(q)} \hat{N}^{(j-1)},$$

$$C = -\sigma_q \tilde{Y}^{(j)} - \sum_{c \neq q} \delta\sigma_c^{(q)} I_c^{(j)T} \tilde{W}_c^{(j-1)} I_c^{(j)} - \dot{Y}^{(j)} \Lambda^{(j)} \dot{Y}^{(j)}. \tag{5.4}$$

Substituting into (5.1) the expression (12.16), given in part I, for the inverse of any matrix of the form (5.3) (and replacing g by $j - 1$) yields the result that (5.1) also

holds when $g=j$, with

$$Q_j=Q_{j-1}-R_{j-1}^T A^{-1}R_{j-1}, \qquad R_j=\sum_{a \neq q} \hat{Y}_a^{(j)T}B_a A^{-1}R_{j-1},$$

$$S_j=\sigma_q I^{(j)}+\sum_{a,b \neq q} \hat{Y}_a^{(j)T}(\delta\sigma_a \tilde{W}_a^{(j-1)}\delta_{ab}-B_a A^{-1}B_b)\hat{Y}_b^{(j)}. \qquad (5.5)$$

Thus we have established that $\sigma_g^*(\Lambda^{(g)})$ is a fractional linear matrix transformation of $\Lambda^{(g)}$ of the form (5.1), and it directly follows that $\sigma_g^*(\hat{N}^{(g)}\Omega^{(g)}\hat{N}^{(g)})$ is a fractional linear matrix transformation of $\Omega^{(g)}$. Furthermore (5.2) and the recursion relations (5.4) and (5.5) can be used to generate the matrix parameters Q_g, R_g, and S_g: there is no need to work with the continued fraction expansion.

From (5.1) and the identity that $(I-A)^{-1}-I=(A^{-1}-I)^{-1}$ for any matrix A, we have the alternative representation

$$\sigma_g^*(\Lambda^{(g)})=Q_g^\dagger+R_g^{\dagger T}(\tilde{\Lambda}^{(g)}+S_g^\dagger)^{-1}R_g^\dagger \qquad (5.6)$$

for $\sigma_g^*(\Lambda^{(g)})$ in terms of the inverse $\tilde{\Lambda}^{(g)}$ of $\Lambda^{(g)}$, where

$$Q_g^\dagger=Q_g-R_g^T S_g^{-1}R_g, \qquad R_g^\dagger=S_g^{-1}R_g, \qquad S_g^\dagger=S_g^{-1}. \qquad (5.7)$$

6. Half-Plane Bounds on Scalar Ω-Functions

To obtain explicit expressions for the various bounds we still need to calculate $\sigma_g^*(\mathcal{S})$ for the appropriate sets

$$\mathcal{S}=\mathcal{S}(k,\mathcal{G}_\theta), \qquad \mathcal{S}(k,\mathcal{W}), \qquad \hat{N}^{(g)}\mathcal{S}(k,\mathcal{G}_{\theta,q})\hat{N}^{(g)}, \qquad \hat{N}^{(g)}\tilde{\mathcal{S}}(k,\mathcal{G}_{\theta,q}^\dagger)\hat{N}^{(g)},$$

or

$$\hat{N}^{(g)}[\mathcal{S}(k,\mathcal{F})\cap\tilde{\mathcal{S}}(k,\mathcal{F}^\dagger)]\hat{N}^{(g)},$$

where $k=dn'^g\equiv d(n-1)^g$. This can be accomplished by identifying the matrices in $\mathcal{S}$ that get mapped onto the boundary of $\sigma_g^*(\mathcal{S})$ in σ^* space and then constructing their image.

For ease of analysis only bounds on scalar Ω-functions are considered: such bounds are especially important because, from Sect. 3, they apply to the diagonal elements of any tensor Ω-function. Following some remarks on a general approach for calculating $\sigma_g^*(\mathcal{S})$ given an arbitrary set $\mathcal{S}$, our focus is on constructing half-plane bounds: wedge bounds are considered in Sect. 7. For these bounds the set $\mathcal{S}$ has a particularly simple characterization. Analytic expressions for the complete hierarchy of half-plane and half-plane reciprocal bounds are derived *and each θ-sequence is found to form a nested sequence of circles in the complex plane*. The remainder of this section covers the question of attainability of the bounds, and deals with the technicalities of constructing their inner hull.

It will be assumed the variables σ_a do not all share the same argument in the complex plane. Otherwise the Wiener-Beran and Hashin-Shtrikman bounds apply and the problem is solved: as discussed in Sect. 4, these bounds are optimal for scalar Ω-functions and correspond to substituting $\Lambda^{(g)}=0$, $\Lambda^{(g)}=\infty I$, $\Lambda^{(g)}=\sigma_L N^{(g)}$ or $\Lambda^{(g)}=\sigma_U N^{(g)}$ in (5.1).

Let us define any infinitesimal variation $\partial\Lambda$ in $\Lambda\in\mathscr{S}$ to be *unconstrained with respect to* $\mathscr{S}$ if both $\Lambda-\partial\Lambda$ and $\Lambda+\partial\Lambda$ lie in the set $\mathscr{S}$. Clearly for scalar Ω-functions, and to first order in $\partial\Lambda$, $\sigma_g^*(\Lambda)$ lies midway on the line in the complex plane joining $\sigma_g^*(\Lambda-\partial\Lambda)$ to $\sigma_g^*(\Lambda+\partial\Lambda)$. This line has slope $\arg\partial\sigma_g^*(\Lambda)$. Hence a necessary, but not sufficient, condition for $\sigma_g^*(\Lambda)$ to lie on the boundary of the set $\sigma_g^*(\mathscr{S})$ is that for every unconstrained variation $\partial\Lambda$ of Λ we have

$$\partial\sigma_g^*(\Lambda)=0, \tag{6.1}$$

or we have

$$\arg\partial\sigma_g^*(\Lambda)=\text{const}\equiv\gamma^0(\text{modulo }\pi) \tag{6.2}$$

to first order in $\partial\Lambda$. When $\sigma_g^*(\Lambda)$ is indeed on the boundary of $\sigma_g^*(\mathscr{S})$ the constant γ^0 which appears in this formula, of course, is the angular slope of the boundary at $\sigma_g^*(\Lambda)$.

For scalar Ω-functions the matrix Q_g that appears in (5.1) is a scalar, Q_g, while R_g is a vector, $\mathbf{R}_g$, in a $k=n'^g$ dimensional space. Substituting (5.1) in (6.1) and (6.2) gives the condition

$$\mathbf{T}^T(\partial\Lambda)\mathbf{T}=0 \quad\text{or}\quad \arg\mathbf{T}^T(\partial\Lambda)\mathbf{T}=\gamma^0, \tag{6.3}$$

where we have introduced the vector

$$\mathbf{T}\equiv(\Lambda+S_g)^{-1}\mathbf{R}_g. \tag{6.4}$$

At fixed γ^0 the set of $\Lambda\in\mathscr{S}$ that satisfy (6.3) for all unconstrained variations $\partial\Lambda$ will get mapped via $\sigma_g^*(\Lambda)$ to a set of points in the complex plane. As γ^0 is varied from 0 to π the points will trace a family of curves, some of which may terminate if the corresponding matrix Λ moves outside $\mathscr{S}$. The set $\sigma_g^*(\mathscr{S})$ will be the region enclosed by the outermost curves in this family.

To implement this scheme consider the $(2g-1)$th order half-plane bounds (4.13) obtained by taking $\mathscr{S}=\mathscr{S}(k,\mathscr{G}_\theta)$, where $k\equiv n'^g$, and θ satisfies (4.1). Any matrix Λ in this set can be parametrized in the form

$$\Lambda=e^{i\theta}(\Lambda'+i\Lambda''), \quad\text{with}\quad \Lambda''\geqq0, \tag{6.5}$$

where Λ' and Λ'' are real symmetric matrices and Λ' (unlike Λ'') need not be positive semidefinite. We will assume that both Λ' and Λ'' have finite eigenvalues: the extreme case where some of the eigenvalues are infinite can be treated separately (see Sect. 7) and does not alter our results.

Since all infinitesimal, symmetric, real variations $\partial\Lambda'$ of Λ' are allowed, (6.3) implies that all elements of the vector $\mathbf{T}$ have the same argument in the complex plane. Hence there exists a real vector $\mathbf{T}_R$ such that

$$\mathbf{T}=e^{i\gamma}\mathbf{T}_R, \tag{6.6}$$

where

$$\gamma=(\gamma^0-\theta)/2 \quad\text{or}\quad (\pi+\gamma^0-\theta)/2. \tag{6.7}$$

By inserting (6.6) back into (6.3), we deduce that

$$\mathbf{T}^T(\partial\Lambda')\mathbf{T}=0 \tag{6.8}$$

for all infinitesimal unconstrained variations $\partial\Lambda''$ of Λ''. So suppose Λ'' has some eigenvector $\mathbf{v}''$ with a non-zero eigenvalue λ''. We are certainly free to increase or decrease λ'', and consequently (6.8) implies

$$\mathbf{v}''^{T}\mathbf{T}=0.\tag{6.9}$$

Now consider the effect of reducing the eigenvalue λ'' by a finite amount, $\delta\lambda''$, to form a new matrix

$$\Lambda^{-}\equiv\Lambda-i\delta\lambda''e^{i\theta}\mathbf{v}''\mathbf{v}''^{T}.\tag{6.10}$$

From (5.1) and (6.9) we have

$$\sigma_{g}^{*}(\Lambda^{-})=\sigma_{g}^{*}(\Lambda)-i\delta\lambda''e^{i\theta}(\mathbf{v}''^{T}\mathbf{T})\left[\mathbf{v}''^{T}(\Lambda^{-}+S_{g})^{-1}\mathbf{R}_{g}\right]=\sigma_{g}^{*}(\Lambda).\tag{6.11}$$

Thus we can reduce the eigenvalues of Λ'' to zero without changing $\sigma_{g}^{*}(\Lambda)$. Therefore it suffices to look for solution of (6.3) with $\Lambda''=0$: when Λ' is positive definite this corresponds to considering those Ω-functions with a terminating set of weights of the form (2.29).

Substituting $\Lambda=e^{i\theta}\Lambda'$ and (6.6) in (6.4) gives,

$$(\Lambda'+e^{-i\theta}S_{g})\mathbf{T}_{R}=e^{-i(\gamma+\theta)}\mathbf{R}_{g}.\tag{6.12}$$

Since $\mathbf{T}_{R}$ and Λ' are both real, we can eliminate Λ' by taking the imaginary part of (6.12) to obtain the result

$$\mathbf{T}_{R}=[\text{Im}(e^{-i\theta}S_{g})]^{-1}\text{Im}(e^{-i(\gamma+\theta)}\mathbf{R}_{g}).\tag{6.13}$$

By defining

$$\mathbf{X}_{g,\theta}\equiv[\text{Im}(e^{-i\theta}S_{g})]^{-1}\mathbf{R}_{g}\quad\text{(for odd-order bounds)},\tag{6.14}$$

and substituting (6.4) into (5.1) we find

$$\sigma_{g}^{*}(\Lambda)=Q_{g}-\mathbf{R}_{g}^{T}\mathbf{T}=Q_{g}-e^{-i\gamma}\mathbf{X}_{g,\theta}^{T}\text{Im}(e^{-i(\gamma+\theta)}\mathbf{R}_{g}),\tag{6.15}$$

for all points Λ such that $\sigma_{g}^{*}(\Lambda)$ is on the boundary of the half-plane bounds. To elucidate the dependence on γ this can be re-expressed as

$$\sigma_{g}^{*}(\Lambda)=Q_{g}+ie^{-i\theta}\mathbf{X}_{g,\theta}^{T}\mathbf{R}_{g}/2-ie^{i(2\gamma+\theta)}\mathbf{X}_{g,\theta}^{T}\bar{\mathbf{R}}_{g}/2,\tag{6.16}$$

where $\bar{\mathbf{R}}_{g}$ denotes the complex conjugate of the vector $\mathbf{R}_{g}$.

Clearly, as γ is varied from 0 to π, $\sigma_{g}^{*}(\Lambda)$ given by (6.16) inscribes a circle in the complex plane. This circle, of radius $\mathbf{X}_{g,\theta}^{T}\bar{\mathbf{R}}_{g}/2$, must contain σ^{*}. The quantities Q_{g}, $\mathbf{R}_{g}$, and S_{g} that enter into the expression (6.16) via (6.14) are given by (5.2) and the recursion relations (5.4) and (5.5). Thus once the geometric parameters are known, (6.16) provides an explicit formula for computing the half-plane bounds to any odd order, for any orientation, θ, of the half-plane.

The even-order half-plane and half-plane reciprocal bounds are determined by similar analysis. Any complex matrix Λ in the set $\mathscr{S}=\hat{N}^{(g)}\mathscr{S}(k,\mathscr{G}_{\theta,q})\hat{N}^{(g)}$, and only those matrices in this set can be represented in the form

$$\Lambda=N^{(g)}\sigma_{q}+e^{i\theta}(\Lambda'+i\Lambda'')\quad\text{with}\quad\Lambda''\geqq0,\tag{6.17}$$

in which Λ' and Λ'' are real and symmetric. Again it suffices to set $\Lambda'' = 0$, and the resulting $(2g)$th-order half-plane bounds retain the form (6.16), but with $\mathbf{X}_{g,\theta}$ replaced by

$$\mathbf{X}_{g,\theta} \equiv [\mathrm{Im}\, e^{-i\theta}(S_g + \sigma_q N^{(g)})]^{-1} \mathbf{R}_g \quad \text{(for even-order bounds)}. \tag{6.18}$$

The $(2g)$th-order half-plane reciprocal bounds (4.24) are easiest to examine using the alternative representation (5.6) of $\sigma_g^*(\Lambda)$. By direct analogy with (6.16) and (6.18) the boundary of $\sigma_g^*(\mathcal{S})$ is described by the circle

$$\sigma_g^*(\Lambda) = Q_g^\dagger - i e^{i\theta} \mathbf{X}_{g,\theta}^{\dagger T} \mathbf{R}_g^\dagger / 2 + i e^{-i(2\gamma + \theta)} \mathbf{X}_{g,\theta}^{\dagger T} \bar{\mathbf{R}}_g^\dagger / 2, \tag{6.19}$$

as γ varies from 0 to π, where

$$\mathbf{X}_{g,\theta}^\dagger \equiv [\mathrm{Im}\, e^{i\theta}(S_g^\dagger + \tilde{N}^{(g)}/\sigma_q)]^{-1} \mathbf{R}_g^\dagger \quad \text{(for even-order bounds)} \tag{6.20}$$

and $\bar{\mathbf{R}}_g^\dagger$ denotes the complex conjugate of $\mathbf{R}_g^\dagger$.

The nesting property of the half-plane bounds, established in Sect. 4 now implies that each θ-sequence of half-plane bounds forms a nested sequence of circles in the complex plane. Similarly each θ-sequence of half-plane reciprocal bounds forms a nested sequence of circles. Taken together, and keeping θ fixed, they result in a nested sequence of bounds comprised of circles, corresponding to the odd-order half-plane bounds, alternating with lens-shaped regions formed by the intersection of the pairs of circles corresponding to the even-order half-plane and half-plane reciprocal bounds.

At certain values of θ, specified below, some sections of circular arc in such a jth-order bound can be attainable. Consider the odd-order bounds, with $j = 2g - 1$, and suppose θ is at its extreme value, $\arg \sigma_p$. In terms of the vector

$$\xi \equiv e^{-i(\gamma + \theta)} \mathbf{R}_g - e^{-i\theta} S_g \mathbf{T}_R, \tag{6.21}$$

which is purely real because $\mathbf{T}_R$ is given by (6.13), the solutions for Λ' of (6.12) take the form

$$\Lambda' = (\mathbf{T}_R^T \cdot \xi)^{-1} \xi \xi^T + \sum_{j=1}^{k-1} b_j \boldsymbol{\eta}_j \boldsymbol{\eta}_j^T, \tag{6.22}$$

where the b_j, $j = 1, 2, ..., k-1$, are a set of arbitrary real constants and then $\boldsymbol{\eta}_j$ are chosen to be any set of $k-1$ orthonormal real vectors satisfying

$$\mathbf{T}_R^T \cdot \boldsymbol{\eta}_j = 0, \quad j = 1, 2, ..., k-1. \tag{6.23}$$

Now if $\Lambda' \geq 0$ and $\theta = \arg \sigma_p$, the matrix $\Lambda = e^{i\theta} \Lambda'$ can be reexpressed in the form (4.9), with $\Lambda_m = 0$ and $\Lambda_p = \Lambda'/|\sigma_p| \geq 0$. When this occurs the corresponding point $\sigma_g^*(\Lambda)$ lying on the circle (6.16) is also on the boundary of the wedge bounds and hence is attainable in the class of Ω-functions. Since the constants b_j in (6.22) can be chosen non-negative, a positive semi-definite matrix solution Λ' exists if and only if the *attainability condition*

$$\mathbf{T}_R^T \cdot \xi \geq 0 \tag{6.24}$$

is met when $\theta = \arg \sigma_p$. By substituting the expressions (6.13) and (6.21) for $\mathbf{T}_R$ and ξ in (6.24) this attainability condition is recast in the form

$$\mathrm{Re}[e^{-i(2\gamma + \theta)} r(\theta)] \geq 1, \tag{6.25}$$

where $r(\theta)$ is the complex ratio

$$r(\theta) \equiv \mathbf{X}_{g,\theta}^T \bar{S}_g \mathbf{X}_{g,\theta} / \{\mathbf{X}_{g,\theta}^T [\mathrm{Re}(e^{-i\theta} S_g)] \bar{\mathbf{X}}_{g,\theta}\}, \tag{6.26}$$

in which $\bar{S}_g$ and $\bar{\mathbf{X}}_{g,\theta}$ are the complex conjugates of S_g and $\mathbf{X}_{g,\theta}$. Thus the bounds (6.16) are attainable at $\theta = \arg \sigma_p$ if and only if $|r(\theta)| \geqq 1$. They are attained on the length of circular arc with endpoints given, from (6.25), by

$$\gamma = \{[\arg r(\theta)] - \theta \pm \cos^{-1}(1/|r(\theta)|)\}/2. \tag{6.27}$$

At the other extreme value of θ, namely $\theta = \pi + \arg \sigma_m$, the bounds are attainable when $\Lambda' \geqq 0$, and this again occurs between those values of γ given by (6.27), provided $|r(\theta)| \geqq 1$. Through similar analysis it follows that the even order half-plane bounds (or half-plane reciprocal bounds) may be attainable at up to n values of θ, namely when θ (or $-\theta$) coincides modulo π, with the angular slope of one of the edges of $\mathscr{F}$ (or of $\mathscr{F}^\dagger$) that joins two adjacent vertices σ_a and σ_b (or $1/\sigma_a$ and $1/\sigma_b$) for some $a, b \in (1, 2, ..., n)$.

The calculation of the inner-hull of the jth order half-plane bounds requires some care. For the odd-order bounds, with $j = 2g - 1$, we first plot the attainable sections of circular arc that occur when $\theta = \arg \sigma_m$ or $-\pi + \arg \sigma_m$. At other values of θ any variation $\partial \theta$ in θ is unconstrained. Differentiating (6.16) with respect to θ gives (after some algebraic manipulation) the result that (6.2) and (6.7) are satisfied when

$$\mathrm{Re}[e^{-i(2\gamma + \theta)} r(\theta)] = 1, \tag{6.28}$$

where $r(\theta)$ is the same factor, defined by (6.26), that occurs in (6.25). Whenever $|r(\theta)| \geqq 1$ this has the solution (6.27) for the angles $\gamma(\theta)$. A pair of curves is generated by substituting (6.27) in the bounds (6.16) and varying θ subject to (4.1) and the constraint $|r(\theta)| \geqq 1$. At $\theta = \arg \sigma_p$ and $\theta = -\pi + \arg \sigma_m$ *these curves clearly meet with the attainable sections of arc (if any) and together they form the closed boundary of the inner hull.*

A similar procedure can be followed to construct the inner hull of the even-order bounds, by first plotting the attainable sections of circular arc (which occur at n or less values of θ) and then by constructing the inner hull at the intermediate values of θ, within the range (4.1). For the $(2g)$th-order half-plane bounds the analogous formulae to (6.21)–(6.28) are obtained by replacing S_g with $S_g + \sigma_q N^{(g)}$. For the $(2g)$th-order half-plane reciprocal bounds it is necessary to change various signs, add daggers to the appropriate symbols and replace $S_g^\dagger$ with $S_g^\dagger + \bar{N}^{(g)}/\sigma_q$.

For scalar Ω-functions of two-variables Λ' is a real scalar, Λ', and there is a 1-1 correspondence between the angles $\gamma \in [0, \pi]$ in (6.16) and values of Λ' along the real line. Hence when $\theta = \arg \sigma_p$ (and when $\theta = -\pi + \arg \sigma_m$) there exists some arc of the circle (6.16), corresponding to $\Lambda' \geqq 0$ (or $\Lambda' \leqq 0$), which is attainable. The pair of attainable arcs meet when $\Lambda' = 0$ and when $\Lambda' = \infty$. Thus the inner hull of the $(2g-1)$th-order bound is an optimal bound and consists merely of a lens-shaped region in the complex plane: when $n = 2$ the curves obtained by substituting (6.27) in (6.16) degenerate into a pair of points at the corners of the lens. A similar argument, based on choosing $\theta = \arg(\sigma_p - \sigma_m)$, establishes the optimality of the inner hull of the even-order half-plane bounds which likewise reduce to lens-shaped regions. The optimality of these bounds implies they are identical to the

nested sequence of lens-shaped regions in the complex plane derived by Milton [22], which in turn correspond to the bounds on Stieltjes functions due to Gragg [48] and Baker [50]. Numerical studies of the bounds for regular arrays of spheres and lattices of cylinders provide dramatic evidence of their utility when the geometric parameters are known: the bounds converge rapidly to the exact value of σ^*, even when the inclusions nearly touch and even at conductivity ratios σ_1/σ_2 as large as 10,000 [23].

7. Wedge Bounds on Scalar Ω-Functions

The wedge bounds on scalar Ω-functions are harder to calculate than the half-plane bounds but deserve attention because they are optimal over the class of Ω-functions. Those sections on the boundary of the wedge bounds $\sigma_g^*(\mathscr{S}(k, \mathscr{W}))$ that do not coincide with the attainable sections of the half-plane bounds are shown here to be generated by matrices $\Lambda \in \mathscr{S}(k, \mathscr{W})$ of the form (4.9), where $\Lambda_m = 0$ and Λ_p has a mixture of only zero and infinite eigenvalues with at most two zero eigenvalues. This result enables us to derive explicit expressions for the optimal set of complex 1st-order bounds on scalar 3-variable Ω-functions. They include the attainable sections of the 1st-order half-plane bounds, which in turn coincide with the bounds on scalar Σ-functions conjectured by Golden and Papanicolaou [53] and rigorously proved in [54]. The remaining segments of the 1st-order wedge bounds are completely new and substantially improve upon the Golden-Papanicolaou bounds. They are not, however, represented by a circle in the complex plane.

Recall that any matrix $\Lambda \in \mathscr{S}(k, \mathscr{W})$ can be represented in the form (4.9) in terms of the matrices Λ_m and Λ_p given by (4.8). If Λ_p has some infinite eigenvalues, then the singular infinite part of Λ_p can be removed and added to Λ_m without influencing the inverse matrix $(S_g + \Lambda)^{-1}$ that determines the wedge bounds $\sigma_g^*(\mathscr{S})$ via (5.1). Hence it suffices to consider those matrices Λ for which Λ_p has finite eigenvalues.

Now assume Λ_m has at least one positive finite eigenvalue with eigenvector $\mathbf{v}_{m,1}$ such that

$$\mathbf{T}^T \cdot \mathbf{v}_{m,1} \neq 0, \tag{7.1}$$

where the vector $\mathbf{T}$ is defined by (6.4). Let $\mathbf{v}_{m,2}, \mathbf{v}_{m,3}, \ldots, \mathbf{v}_{m,h}$ and $\mathbf{v}_{m,h+1}, \mathbf{v}_{m,h+2}, \ldots, \mathbf{v}_{m,k}$ denote the two groups of remaining eigenvectors that have finite non-negative (possibly zero) eigenvalues and infinite eigenvalues, respectively: here h denotes the number of finite eigenvalues of Λ_m. For any two real infinitesimals ε and ε' and for any integer j with $h \geq j \geq 2$, the variation

$$\partial \Lambda_m = \varepsilon \mathbf{v}_{m,1} \mathbf{v}_{m,1}^T + \varepsilon'(\mathbf{v}_{m,1} \mathbf{v}_{m,j}^T + \mathbf{v}_{m,j} \mathbf{v}_{m,1}^T) \tag{7.2}$$

is an unconstrained variation of Λ_m, and hence from (6.3) and (7.1) we have

$$\mathbf{T}^T \cdot \mathbf{v}_{m,i} = 0 \quad \text{or} \quad \arg(\mathbf{T}^T \cdot \mathbf{v}_{m,i}) = \gamma, \quad \forall i \leq h, \tag{7.3}$$

where (6.7) defines γ. For those eigenvectors with infinite eigenvalues the formula (6.4) for $\mathbf{T}$ in terms of Λ directly implies that $\mathbf{T}^T \cdot \mathbf{v}_{m,i} = 0$ for all $i > h$. Hence $\mathbf{T}$ can be expressed in the form (6.6), where $\mathbf{T}_R$ is real. From the argument developed in (6.8)–(6.11), it clearly suffices to consider those matrices $\Lambda = \sigma_m \Lambda_m$, with $\Lambda_p = 0$.

Similar analysis shows that $\sigma_g^*(\Lambda)$ remains constant when Λ_m is increased by, say, the finite amount

$$\delta\Lambda_m = \sum_{j=1}^{k-1} \boldsymbol{\eta}_j \boldsymbol{\eta}_j^T, \tag{7.4}$$

where the $(k-1)$ orthonormal real vectors $\boldsymbol{\eta}_j$ are chosen to satisfy $\mathbf{T}_R^T \cdot \boldsymbol{\eta}_j = 0$. Since $\mathbf{T}_R^T \cdot \mathbf{v}_{m,1} \neq 0$, this increase (7.4) will produce a new positive definite matrix Λ_m^+ with non-zero eigenvalues.

Thus if the boundary of $\sigma_g^*(\mathscr{S})$ is attained for some matrix $\Lambda \equiv \sigma_m \Lambda_m \in \mathscr{S}$ such that Λ_m has at least one non-zero eigenvalue with eigenvector $\mathbf{v}_{m,1}$ satisfying (7.1), then there exists another strictly positive definite matrix $\Lambda^+ \equiv \sigma_m \Lambda_m^+ \in \mathscr{S}$, attaining the same value $\sigma_g^*(\Lambda^+) = \sigma_g^*(\Lambda)$ on the bounds. The inverse matrix $\tilde{\Lambda}^+$ will now be bounded. By repeating the argument in the representation (5.6), we subsequently obtain a bounded strictly positive definite matrix Λ_m^{++} such that

$$\Lambda^{++} \equiv \sigma_m \Lambda_m^{++} \in \mathscr{S}, \qquad \sigma_g^*(\Lambda^{++}) = \sigma_g^*(\Lambda). \tag{7.5}$$

Any infinitesimal variation $\partial\Lambda_m^{++}$ in Λ_m^{++} is unconstrained and therefore $\sigma_g^*(\Lambda^{++})$, or equivalently $\sigma_g^*(\Lambda)$, must lie on the boundary of the $(2g-1)$th-order *half-plane* bounds.

To obtain the sections on the boundary of $\sigma_g^*(\mathscr{S}(k, \mathscr{W}))$ that do not coincide with the half-plane bounds, we clearly need to consider matrices $\Lambda \in \mathscr{S}(k, \mathscr{W})$ such that $\mathbf{T}^T \cdot \mathbf{v}_m = 0$ for all eigenvectors $\mathbf{v}_m$ of Λ_m that have positive finite eigenvalues. Since these eigenvalues can be reduced to zero without changing $\sigma_g^*(\Lambda)$ [see (6.9–11)] it suffices to restrict attention to matrices Λ for which Λ_m has only zero and infinite eigenvalues. The singular infinite part of Λ_m can be shifted to Λ_p without altering $\sigma_g^*(\Lambda)$ (leaving $\Lambda_m = 0$) and the above argument, with the roles of Λ_m and Λ_p interchanged, then implies that we need only consider matrices Λ_p with zero and infinite eigenvalues. This corresponds to an Ω-function terminated by a normalization factor with only zero and infinite eigenvalues.

We are still free to increase Λ_p by the finite amount

$$\delta\Lambda_p = \sum_{j=1}^{k-2} b\boldsymbol{\eta}_j \boldsymbol{\eta}_j^T, \tag{7.6}$$

where b is any positive real constant and the $k-2$ orthonormal real vectors $\boldsymbol{\eta}_j$ are chosen to satisfy

$$(\mathrm{Re}\,\mathbf{T}^T) \cdot \boldsymbol{\eta}_j = (\mathrm{Im}\,\mathbf{T}^T) \cdot \boldsymbol{\eta}_j = 0. \tag{7.7}$$

By taking the limit $b \to \infty$, we conclude that *it is sufficient to take matrices* $\Lambda = \sigma_p \Lambda_p$, *such that* Λ_p *has at most two zero eigenvalues with the remaining eigenvalues being infinite*. When Λ_p has only one zero eigenvalue with eigenvector $\mathbf{v}_1$, then (5.1) takes the form

$$\sigma_g^*(\Lambda) = Q_g - (\mathbf{v}_1^T \cdot \mathbf{R}_g)^2 (\mathbf{v}_1^T S_g \mathbf{v}_1)^{-1}, \tag{7.8}$$

and when there are two zero eigenvalues, with eigenvectors $\mathbf{v}_1$ and $\mathbf{v}_2$, we have

$$\sigma_g^*(\Lambda) = Q_g - \mathbf{R}_g^T \nu (\nu^T S_g \nu)^{-1} \nu^T \mathbf{R}_g, \tag{7.9}$$

where ν is the $2 \times k$ dimensional matrix with columns $\mathbf{v}_1$ and $\mathbf{v}_2$. The best choice for the normalized eigenvectors $\mathbf{v}_1$ and $\mathbf{v}_2$ can in principle be determined from the condition (7.2), which must hold to first order in any variations in the orientations of these eigenvectors. In practice, however, it may be easier to numerically evaluate (7.8) and (7.9) over the complete range of orientations of $\mathbf{v}_1$ and $\mathbf{v}_2$. The resulting outermost curve together with the attainable sections of (7.16) forms the boundary of the wedge bounds.

To provide a concrete example, we now specialize to the first-order wedge bounds on scalar 3-variable Ω-functions. (We then have $g = 1$, $d = 1$ and $n = 3$.) Given any angle $\varrho \in [0, 2\pi]$ let us define a unit vector $\boldsymbol{\alpha}(\varrho)$ with components $(\cos\varrho, \sin\varrho)$ and select

$$\mathbf{v}_1 = \dot{Y}^{(1)} \boldsymbol{\alpha} \tag{7.10}$$

as the eigenvector of Λ_p that has a zero eigenvalue. Note that $\mathbf{v}_1$, which has not been normalized, takes all possible orientations as ϱ is varied from 0 to 2π. Substituting (7.10) and (5.2) in the bounds (7.8) and taking σ_3 as our reference variable yields the expression

$$\sigma_g^*(\Lambda) = f_1 \sigma_1 + f_2 \sigma_2 + f_3 \sigma_3 - \frac{[\sigma_1 \cos\varrho + \sigma_2 \sin\varrho - \sigma_3(\cos\varrho + \sin\varrho)]^2}{(\sigma_1/f_1)\cos^2\varrho + (\sigma_2/f_2)\sin^2\varrho + (\sigma_3/f_3)(\cos\varrho + \sin\varrho)^2} \tag{7.11}$$

which generates a closed curve, parametrized by ϱ. All points along this curve are attainable, but not all portions of it contribute to the boundary of the wedge bounds. There are no contributions from the other formula (7.9) because it only generates a single point $\sigma_g^*(\Lambda)$ with $\Lambda = 0$. Curiously, the curve (7.11) degenerates to an arc of a circle (but not a complete circle) in the complex plane when a pair of the component conductivities σ_1, σ_2 or σ_3 become equal, or in the limit in which one of the volume fractions f_1, f_2 or f_3 becomes vanishingly small.

To obtain the remaining sections on the boundary of the wedge bounds we need to evaluate the half-plane bounds at the extreme values $\theta = \arg\sigma_p$ and $\theta = -\pi + \arg\sigma_m$. Although this can be achieved by direct substitution of (5.2) in (6.16), let us follow a different approach to elucidate the connection with the work of Golden and Papanicolaou [53, 55].

Recall from Sect. 5 that the first-order half-plane bounds with $\arg\theta = \sigma_p$ can be generated from $\sigma_1^*(\sigma_p\Lambda_p)$ as Λ_p varies over all real symmetric 2×2 matrices. Equivalently, from (2.20) and (4.2) we can take σ_p as our reference medium and vary $\Delta_{a,b}^{+(p)}$ over 2×2 complex matrices of the form

$$\Delta_{a,b}^{+(p)} = D_{a,b}^{(p)} - \delta_{ab} s_a^{(p)}, \tag{7.12}$$

where $D_{a,b}^{(p)}$ is any real symmetric 2×2 matrix. Because of the degeneracy (6.22) of the matrices $\Lambda = e^{i\theta}\Lambda' = \sigma_p\Lambda_p$ that attain any given point $\sigma_1^*(\Lambda)$ on the boundary of the half-plane bounds, it suffices to consider diagonal matrices $D_{a,b}^{(p)} = \delta_{ab}\lambda_a^{(p)}$. This results, via (7.12), (2.23), and (2.11), in a conductivity

$$\sigma_1^*(\Lambda) = \sigma_p \left[1 - \sum_{a \neq p} \frac{f_a}{\lambda_a^{(p)} - s_a^{(p)}} \right], \tag{7.13}$$
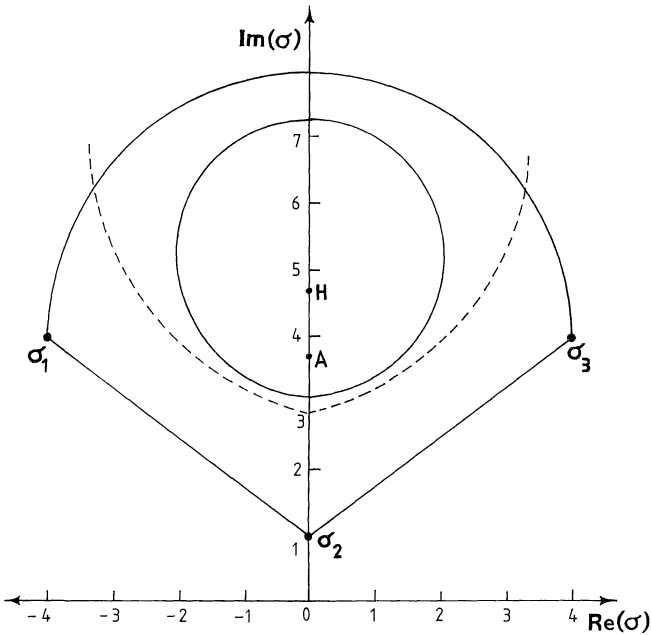
Fig. 2. The scalar elementary polygon bounds (outermost solid curve) and the scalar 1st-order wedge bounds (innermost solid curve) for the example chosen by Golden and Papanicolaou of a three component composite with complex component conductivities $\sigma_1 = -4+4i$, $\sigma_2 = i$, and $\sigma_3 = 4+4i$ and volume fractions $f_1 = 9/20$, $f_2 = 1/10$, and $f_3 = 9/20$. These bounds enclose the diagonal elements of the effective conductivity tensor, σ^*. The curve (7.11) forms the complete boundary of the wedge bounds: no contribution comes from the Golden-Papanicolaou bounds which are shown here as dashed lines forming two circular arcs meeting at the imaginary axis. The arithmetic and harmonic means of the local conductivity are represented by points A and H respectively

which is of the form postulated by Golden and Papanicolaou [53, 55]. By following their analysis and optimizing over the two diagonal elements $\lambda_a^{(p)}$, where a takes the values 1 through 3 excluding $a=p$, we obtain the expression

$$\sigma_1^*(\Lambda) = \sigma_p \left[1 + (i+c)^{-1} \sum_{a \neq p} f_a / \mathrm{Im}\, s_a^{(p)} \right], \tag{7.14}$$

for the 1st-order half-plane bounds (6.16) parametrized by the real variable $c \in (-\infty, +\infty)$: as c is varied $\sigma_1^*(\Lambda)$ given by (7.14) traces a circle in the complex plane that contains σ^*. The other extreme half-plane bound, with $\theta = -\pi + \arg \sigma_m$, is obtained simply by replacing p by m in the above formula.

These bounds of Golden and Papanicolaou have also been rigorously established using an extension of the trajectory method of Bergman [54]. In conjunction with (7.11) they complete the boundary of the 1st-order wedge bounds on scalar 3-variable Ω-functions: the curve (7.11) meets tangentially with the attainable circular arcs of the half-plane bounds. Note the bounds (7.11) and (7.14) still depend on σ_p in the limit as $f_p \to 0$. This strongly suggests they can be improved
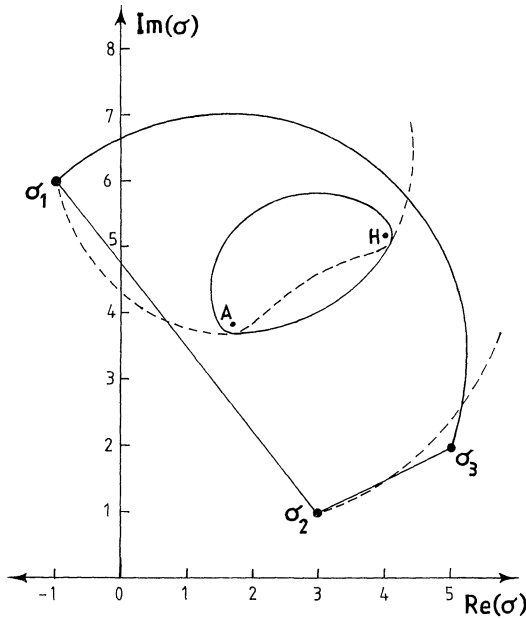
Fig. 3. For a different choice of component conductivities, $\sigma_1 = -1 + 6i$, $\sigma_2 = 3 + i$, and $\sigma_3 = 5 + 2i$, and volume fractions, $f_1 = 1/2$, $f_2 = 1/3$, and $f_3 = 1/6$, one circular arc of the Golden-Papanicolaou bounds (7.14) contributes to the boundary of the scalar 1st-order wedge bounds: its analytical continuation is the dashed arc passing through σ_1. The other Golden-Papanicolaou bound, shown here as a dashed arc passing through σ_2 only marginally improves upon the outermost elementary polygon bounds because the origin, σ_2 and σ_3 are almost colinear. In the limit in which σ_2 equals σ_3 the bounds merge into the lens shaped region appropriate for two-component composites. The dashed line inside the wedge bounds represents the analytic continuation of the curve (7.11)

when applied to the diagonal elements of conductivity tensors of three-component composites. However, the bounds *are* optimal over the class of Ω-functions.

Three examples of these 1st-order wedge bounds are graphed in Figs. 2–4. In Fig. 2, corresponding to the example chosen by Golden [28, 55], the half-plane bounds do not contribute to the wedge bounds while in Figs. 3 and 4 one arc and two arcs, respectively, contribute and meet tangentially with the curve generated from (7.11). The improvement gained over the Golden-Papanicolaou half-plane bounds is clearly substantial in both Figs. 2 and 3.

8. Convergence of the Bounds

The proof that the jth-order wedge-polygon bounds and the jth-order half-plane and half-plane reciprocal bounds converge in the limit $j \to \infty$ (i.e. as progressively more information is specified about the Ω-function) is based on the extension of Bergman's trajectory method [54]. The idea is to parametrize the given set of component conductivities σ_a, $a = 1, 2, \ldots, n$, in terms of a complex variable z taking the value z_0, with $\text{Im} z_0 > 0$: the parametrization, and a fixed reference conductivity
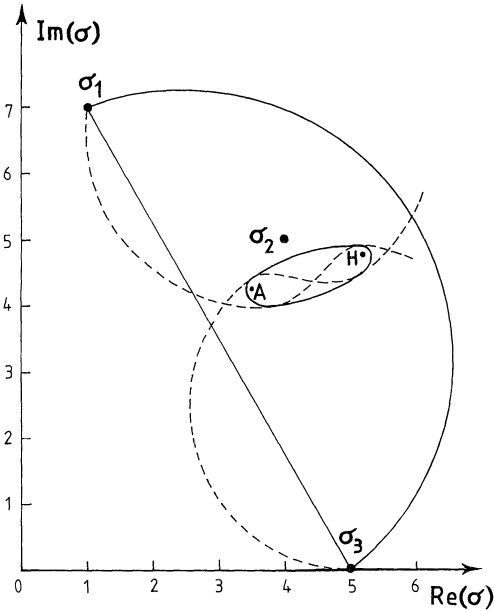
Fig. 4. For component conductivities $\sigma_1 = 1 + 7i$, $\sigma_2 = 4 + 5i$, and $\sigma_3 = 5$ and volume fractions $f_1 = 1/4$, $f_2 = 1/2$, and $f_3 = 1/4$ both arcs of the Golden-Papanicolaou bounds contribute to the wedge bounds. The curve (7.11), whose analytic continuation inside the wedge bounds is denoted by a dashed curve, forms a figure eight

$\sigma_0 (\neq \sigma_a$ for any a), are chosen so the ratios σ_a/σ_0 remain in the upper half of the complex plane as z is varied throughout the upper half plane and take real positive values when z is real and positive. This leads to a parametrization of any point $\sigma_g^*(\Lambda) = \sigma_g^*(z)$ on the $(2g + 1)$th-order bounds in terms of z that ensures $\mathrm{Im}\,[\sigma_g^*(z)/\sigma_0] > 0$ when $\mathrm{Im}\,z > 0$. The convergence of bounds on such single variable functions (as successively more coefficients in the series expansion of $\sigma_g^*(z)/\sigma_0$ in powers of z are incorporated in the bounds) implies the convergence of our bounds on multivariate Ω-functions.

Since the wedge-polygon bounds are more restrictive than the corresponding half-plane or half-plane reciprocal bounds (at any orientation θ of the half-plane) we need only consider the convergence of θ-sequences of half-plane bounds. Not every such θ-sequence is convergent. For example, when the variables σ_a, $a = 1, 2, \ldots, n$ are all real and θ approaches zero from below the successive half-plane bounds merge into each other and do not converge: they only imply $\mathrm{Im}\,\sigma^* \geq 0$. To exclude this possibility we assume θ does not attain the limits (4.1).

It suffices to focus on the convergence, at fixed θ, of the *odd-order* half-plane bounds on *scalar* Ω-functions. Once this convergence is established the even order half-plane and half-plane reciprocal bounds must similarly converge because they are interlaced with the odd-order half-plane bounds. Since the diagonal elements of any tensor Ω-function are scalar Ω-functions (see Sect. 3), the convergence of the half-plane bounds to these diagonal elements in any orthonormal basis set $\mathbf{x}_\ell$, $\ell = 1, 2, \ldots, d$, is ensured and this implies the convergence of the half-plane bounds on tensor Ω-functions.

Given a set of finite variables σ_a, $a = 1, 2, \ldots, n$, in one half of the complex plane, let us parametrize them in the form

$$\sigma_a = \sigma_0 \{1 + z c_a' / [1 + c_a(z+1)]\}, \tag{8.1}$$

where σ_0 is a complex variable, while the constants c_a and c_a' are real satisfying

$$0 < c_a < 1, \quad 0 < c_a' < 1 \quad \forall a, \tag{8.2}$$

and z takes a finite complex value z_0 such that

$$\operatorname{Im} z_0 > 0 \quad \text{and} \quad \arg z_0 = \theta - \arg \sigma_0. \tag{8.3}$$

This ensures, for each component a, that σ_a is a two-variable scalar Ω-function of σ_0 and $(1+z)\sigma_0$. Already it is necessary to assume θ does not attain the limits (4.1): otherwise it is impossible to find a z_0 satisfying (8.3).

As the constants c_a and c_a' are varied over their domain (8.2) of permitted values, σ_a given by (8.1) fills the lens-shaped region of the complex plane, $\mathscr{L}(\sigma_0, (1+z_0)\sigma_0)$, that is bounded on one side by the straight line linking σ_0 to $(1+z_0)\sigma_0$ and on the other side by the circular arc joining these two points that when extended passes through the origin. Clearly σ_0 and z_0 must be chosen so all the points $\sigma_1, \sigma_2, \ldots, \sigma_n$ lie inside $\mathscr{L}(\sigma_0, (1+z_0)\sigma_0)$: this is always possible because as say z_0 approaches infinity while keeping $\arg z_0 = \theta - \arg \sigma_0$ fixed, $\mathscr{L}$ fills a wedge in the complex plane (not containing the origin) that has boundaries meeting at σ_0 at angular slopes of θ and $\arg \sigma_0$.

Recall from Sect. 6 that the $(2g-1)$th-order half-plane bounds are expressible in terms of $\sigma_g^*(e^{i\theta} \Lambda')$ where the matrix Λ', given by (6.22), is real. Since z_0 satisfies (8.3) the associated matrix

$$\Lambda_0 \equiv e^{i\theta} \Lambda' / \sigma_0 z_0 \tag{8.4}$$

is real. Now consider the analytic properties of $\sigma_g^*(z) \equiv \sigma_g^*(\sigma_0 z \Lambda_0)$ as a function of z, while keeping σ_0, θ, the constants c_a and c_a', the geometric parameters and Λ_0 fixed. This function depends on z not only through the term $\sigma_0 z \Lambda_0$, but also through the variables $\sigma_a(z)$ given by (8.1) which enter in the continued fraction expansion for $\sigma_g^*(\Lambda^{(g)})$. From the same type of inductive reasoning given in (3.6–15) we deduce

$$\operatorname{Im}[\sigma_g^*(z) / \sigma_0] \geqq 0 \quad \text{when} \quad \operatorname{Im} z \geqq 0, \tag{8.5}$$

and similarly, for real z, we have

$$\sigma_g^*(z) / \sigma_0 > 0 \quad \text{when} \quad \Lambda_0 = 0 \quad \text{and} \quad z > 1. \tag{8.6}$$

Further elementary analysis shows that

$$\sigma_g^*(\bar{z}) / \sigma_0 = \overline{\sigma_g^*(z) / \sigma_0}, \tag{8.7}$$

where the bar denotes complex conjugation.

Therefore $1 - \sigma_g^*(z) / \sigma_0$ is a real-symmetric function of $1/z$ that maps the upper half plane into the upper half plane, taking the value zero at $z = 1$. Consequently

$$\hbar_g(z) \equiv -(1/z)[1 - \sigma_g^*(z) / \sigma_0] \tag{8.8}$$

is a *Hamburger function* of z, as defined in [51]. Furthermore when $\Lambda_0 = 0$ (8.6) implies that $\hbar_g(z)$ in fact represents a Stieltjes function of z with a radius of convergence around the origin of at least 1.

Now the coefficients in the series expansion

$$\hbar_g(z) = \sum_{i=0}^{\infty} a_i^{(g)} z^i \tag{8.9}$$

for $\hbar_g(z)$ can be evaluated by substituting (8.1) into the continued fraction expansion for $\sigma_g^*(\Lambda^{(g)})$ obtained via (2.16) and (2.17) and (4.2). Since $\delta\sigma_a$ is proportional to z the coefficients $a_i^{(g)}$, for i up to $2g-2$ are expressible in terms of the weights $W_a^{(j)}$ and the normalization factors $N^{(j)}$ with $j \leq g-1$: unlike the higher order coefficients; they neither depend on g nor on the matrix Λ_0.

When $\Lambda_0 = 0$ the coefficients $a_i^{(g)} = a_i^{(\infty)}$, for $i \leq 2g-1$, are associated with a Stieltjes series converging in the unit disk, i.e. they represent *Hausdorff moments* [51]. Consequently the Hamburger moment problem associated with the moments $a_i^{(\infty)}$, $i = 0, 1, 2, \ldots, \infty$ is determinant and the nested sequence of circles [45, 46] that forms a hierarchy of bounds on the Hamburger function $\hbar_\infty(z)$ geometrically converges to a point for all z with $\text{Im}(z) \neq 0$. In this hierarchy the $(2g-2)$th-order bounds that incorporate the moments $a_i^{(\infty)} = a_i^{(g)}$ for $i \leq 2g-2$, apply to any Hamburger function sharing these $2g-1$ moments. In particular the bounds must encircle $\hbar_g(z) = \hbar_g(z, \Lambda_0)$ for all real matrices Λ_0. By setting $z = z_0$ and taking the limit $g \to \infty$, we conclude that $\hbar_g(z_0, \Lambda_0)$ converges to $\hbar_\infty(z_0)$.

Thus at fixed θ the radius $\mathbf{X}_{g,\theta} \bar{\mathbf{R}}_g^T/2$ of the circle (6.16) associated with the $(2g-1)$th-order half-plane bounds converges geometrically to zero: each θ-sequence of half-plane or half-plane reciprocal bounds converges whenever $\theta \neq \arg\sigma_p$ or $-\pi + \arg\sigma_m$. The convergence of the wedge-polygon, half-plane and half-plane reciprocal bounds on tensor Ω-functions is thereby established.

This, incidentally, serves to prove the interchangeability of the limit $h \to \infty$ and the minimum over α in the variational expression for σ^* given in (11.6) of I. By interchanging limits we effectively replaced σ^* by the limit as $h \to \infty$ of the $(2h-1)$th-order upper Beran bound, $\sigma_h^*(\infty I)$, and the equivalence of these two quantities has just been confirmed.

Appendix 1: Convexity of the Class of Ω-Functions

The class of Ω-functions is convex in the sense that if we take two n-variable Ω-functions $'\sigma^*(\sigma_1, \sigma_2, \ldots, \sigma_n)$ and $''\sigma^*(\sigma_1, \sigma_2, \ldots, \sigma_n)$, then the weighted arithmetic average

$$\sigma^* = '\sigma^* c + ''\sigma^*(1-c), \quad \text{for any} \quad 0 < c < 1, \tag{A1.1}$$

is an Ω-function. Since the inverse of an Ω-function is an Ω-function of the reciprocal variables, this immediately implies that the weighted harmonic mean of two Ω-functions is an Ω-function.

To establish this result let $'\mathscr{H}$ and $''\mathscr{H}$ denote the two Hilbert spaces that are associated with the allowable geometric parameters in the continued fraction expansions for $'\sigma^*$ and $''\sigma^*$. More generally we let $'x_\ell$, $'\chi_a$, $'\Gamma_i$, $'\mathscr{P}_a$, $'\mathscr{U}$, $'\mathscr{E}$, and $'\mathscr{J}$ denote the elementary vectors, projection operators and subspaces associated with

$\mathcal{H}$, while the corresponding quantities associated with $''\mathcal{H}$ will be denoted by a pair of inverted commas.

Now consider the Hilbert space

$$\mathcal{H}' = '\mathcal{H} \oplus ''\mathcal{H}, \tag{A1.2}$$

with the standard inner product

$$\langle \mathbf{P}|\mathbf{P}\rangle = \langle 'I\mathbf{P}|'I\mathbf{P}\rangle + \langle ''I\mathbf{P}|''I\mathbf{P}\rangle, \tag{A1.3}$$

in which $'I$ and $''I$ are projection operators onto $'\mathcal{H}$ and $''\mathcal{H}$: this ensures that $'\mathcal{H}$ is orthogonal to $''\mathcal{H}$. Given any constant $c \in (0, 1)$ we define in $\mathcal{H}'$ the orthonormal elementary vectors,

$$\mathbf{x}_\ell = '\mathbf{x}_\ell c^{1/2} + ''\mathbf{x}_\ell (1-c)^{1/2}, \quad \ell = 1, 2, ..., d, \tag{A1.4}$$

the (self-adjoint) projection operators,

$$\chi_a = '\chi_a + ''\chi_a, \quad a = 1, 2, ..., d, \tag{A1.5}$$

$$\Gamma_0 = \sum_{\ell=1}^{d} |\mathbf{x}_\ell\rangle \langle \mathbf{x}_\ell|, \tag{A1.6}$$

$$\Gamma_1 = '\Gamma_1 + ''\Gamma_1, \tag{A1.7}$$

$$\Gamma_2 = '\Gamma_2 + ''\Gamma_2 + '\Gamma_0 + ''\Gamma_0 - \Gamma_0, \tag{A1.8}$$

and the subspaces $\mathcal{P}'_a$, $\mathcal{U}$, $\mathcal{E}'$, and $\mathcal{J}'$ onto which these operators project.

The choice of the elementary vectors and the above operators is motivated by what happens when two isotropic composites are laminated together in proportions c and $1-c$, with layer spacing much larger than the scale of inhomogeneities in each composite. When the field is directed parallel to the layers the effective conductivity in that direction is just a weighted average of the effective conductivities of the two constituent composites and the operators satisfy equations like (A1.5–8).

Alternatively we may regard (A1.4–8) as resulting from three separate operations. First, $\mathcal{U}$, $\mathcal{E}'$, $\mathcal{J}'$, and $\mathcal{P}'_a$ are each taken as the direct sum of the corresponding subspaces in $'\mathcal{H}$ and $''\mathcal{H}$, and the union of the two sets of vectors $'\mathbf{x}_\ell$, $\ell = 1, 2, ..., d$, and $''\mathbf{x}_k$, $k = 1, 2, ..., d$, is chosen as a basis set for $\mathcal{U}$. This gives a $2d$-dimensional block-diagonal effective tensor σ^* with matrices $'\sigma^*$ and $''\sigma^*$ along the diagonal. Next a new basis of vectors for $\mathcal{U}$ is chosen, comprised of the vectors $\mathbf{x}_\ell$ defined via (A1.4) together with the orthogonal set $\mathbf{x}_{\ell+d} \equiv '\mathbf{x}_\ell(1-c)^{1/2} - ''\mathbf{x}_\ell c^{1/2}$, for $\ell = 1, 2, ..., d$. This rotation produces a matrix σ^* with linear combinations of $'\sigma^*$ and $''\sigma^*$ along the block diagonal. Finally, in accordance with (3.17) and (3.18), $\mathcal{U}$ is redefined as the subspace spanned by the vectors $\mathbf{x}_\ell$, $\ell = 1, 2, ..., d$, and $\mathcal{J}'$ is redefined as the direct sum of $'\mathcal{J}$, $''\mathcal{J}$ and the subspace spanned by the remaining vectors $\mathbf{x}_{\ell+d}$, $\ell = 1, 2, ..., d$. This produces a truncated matrix σ^* of the form (A1.1).

To directly check (A1.1) follows from (A1.4–8) note first that any operators $'A$ and $''B$ projecting onto subspaces of $'\mathcal{H}$ and $''\mathcal{H}$ satisfy $'A|''\mathbf{P}\rangle = 0$ and $''B|'\mathbf{P}\rangle = 0$ for all $|''\mathbf{P}\rangle \in ''\mathcal{H}$ and $|'\mathbf{P}\rangle \in '\mathcal{H}$, and hence we have

$$'A''B = ''B'A = 0. \tag{A1.9}$$

Consequently the operators χ_a satisfy the identities (2.1): the subspaces $\mathscr{P}'_a$, $a = 1, 2, \ldots, n$, are mutually orthogonal. Now although Γ_0 cannot be expressed in terms of the operators

$$'\Gamma_0 = \sum_{\ell=1}^{d} |'\mathbf{x}_\ell\rangle \langle '\mathbf{x}_\ell|, \qquad ''\Gamma_0 = \sum_{\ell=1}^{d} |''\mathbf{x}_\ell\rangle \langle ''\mathbf{x}_\ell| \tag{A1.10}$$

that project onto $'\mathscr{U}$ and $''\mathscr{U}$ we nevertheless have the commutation relations.

$$\begin{aligned} \Gamma_0('\Gamma_0 + ''\Gamma_0) &= \Gamma_0 = ('\Gamma_0 + ''\Gamma_0)\Gamma_0, \\ \Gamma_0'\Gamma_0\Gamma_0 &= c\Gamma_0, \qquad \Gamma_0''\Gamma_0\Gamma_0 = (1-c)\Gamma_0, \end{aligned} \tag{A1.11}$$

which follow from (A1.4), (A1.10) and the orthogonality of $'\mathscr{U}$ and $''\mathscr{U}$.

Likewise the orthogonality of the elementary vectors $'\mathbf{x}_\ell$ and $''\mathbf{x}_\ell$ to $'\mathscr{E}$, $''\mathscr{E}$, $'\mathscr{J}$, and $''\mathscr{J}$ implies

$$'\Gamma_i\Gamma_0 = \Gamma_0'\Gamma_i = ''\Gamma_i\Gamma_0 = \Gamma_0''\Gamma_i = 0, \quad \text{for} \quad i = 1 \text{ or } 2. \tag{A1.12}$$

Using these relations it is easy to check that the operators Γ_j, $j = 0, 1, 2$, given by (A1.6)–(A1.8) satisfy the operator identities (2.1): the subspaces $\mathscr{U}$, $\mathscr{E}'$, and $\mathscr{J}'$ are mutually orthogonal.

The whole analysis of I can now be applied to the Hilbert space $\mathscr{H}'$. Field hierarchies $\mathbf{E}_\tau^0$, $\mathbf{J}_\tau^0$ and $\mathbf{P}_{a\tau}^0$ are defined from the recursive relations (2.3) and (2.5). These fields span subspaces $\mathscr{E}$, $\mathscr{J}$, and $\mathscr{P}_a$ of $\mathscr{E}'$, $\mathscr{J}'$, and $\mathscr{P}'_a$, respectively. From (A1.4), (A1.5), and (A1.7) we have the simple identities

$$\mathbf{E}_\tau^0 = '\mathbf{E}_\tau^0 + ''\mathbf{E}_\tau^0, \qquad \mathbf{P}_\tau^0 = '\mathbf{P}_\tau^0 + ''\mathbf{P}_\tau^0, \tag{A1.13}$$

where $'\mathbf{E}_\tau^0$, $'\mathbf{P}_\tau^0$, $''\mathbf{E}_\tau^0$, and $''\mathbf{P}_\tau^0$ are the field hierarchies associated with $'\mathscr{H}$ and $''\mathscr{H}$. By constructing the basis fields $\mathbf{E}_\tau^{(q)}$, $\mathbf{J}_\tau^{(q)}$, and $\mathbf{P}_{a\tau}^{(q)}$, calculating the fundamental geometric parameters N and W_a (in terms of say $'N$, $''N$, $'W_a$, and $''W_a$), we obtain a continued fraction expansion for the effective tensor $\sigma^*(\sigma_1, \sigma_2, \ldots, \sigma_n)$ associated with the Hilbert space $\mathscr{H}'$. This matrix-valued function is clearly an Ω-function.

It remains to show that σ^* is the weighted average of $'\sigma^*$ and $''\sigma^*$. Suppose we are given an arbitrary vector $\mathbf{e} \in \mathscr{U}$, represented in the form

$$\mathbf{e} = '\mathbf{e} + ''\mathbf{e}, \quad \text{where} \quad '\mathbf{e} = '\Gamma_0\mathbf{e} \in '\mathscr{U} \quad \text{and} \quad ''\mathbf{e} = ''\Gamma_0\mathbf{e} \in ''\mathscr{U}. \tag{A1.14}$$

Next define the vectors

$$'\mathbf{j} = '\sigma^*\mathbf{e} \in '\mathscr{U}, \qquad ''\mathbf{j} = ''\sigma^*\mathbf{e} \in ''\mathscr{U}, \tag{A1.15}$$

and let $'\mathbf{J}^* \in '\mathscr{J}$, $'\mathbf{E}^* \in '\mathscr{E}$, $''\mathbf{J}^* \in ''\mathscr{J}$, and $''\mathbf{E}^* \in ''\mathscr{E}$ denote the solutions to the field equations,

$$|'\mathbf{j} + '\mathbf{J}^*\rangle = \sum_{a=1}^{n} \sigma_a'\chi_a|'\mathbf{e} + '\mathbf{E}^*\rangle, \tag{A1.16}$$

$$|''\mathbf{j} + ''\mathbf{J}^*\rangle = \sum_{a=1}^{n} \sigma_a''\chi_a|''\mathbf{e} + ''\mathbf{E}^*\rangle. \tag{A1.17}$$

On the basis of (A1.11) and (A1.15) it follows that

$$\begin{aligned} |\mathbf{j}\rangle \equiv \Gamma_0|'\mathbf{j} + ''\mathbf{j} + '\mathbf{J}^* + ''\mathbf{J}^*\rangle &= \Gamma_0|'\mathbf{j} + ''\mathbf{j}\rangle = \Gamma_0'\Gamma_0\Gamma_0|'\sigma^*\mathbf{e}\rangle + \Gamma_0''\Gamma_0\Gamma_0|''\sigma^*\mathbf{e}\rangle \\ &= (c'\sigma^* + (1-c)''\sigma^*)|\mathbf{e}\rangle, \end{aligned} \tag{A1.18}$$

and (A1.18) implies

$$|\mathbf{J}^*\rangle \equiv \Gamma_2|'\mathbf{j} + ''\mathbf{j} + '\mathbf{J}^* + ''\mathbf{J}^*\rangle = |'\mathbf{j} + ''\mathbf{j} + '\mathbf{J}^* + ''\mathbf{J}^*\rangle - |\mathbf{j}\rangle. \qquad (A1.19)$$

By defining

$$|\mathbf{E}^*\rangle = \Gamma_1|'\mathbf{e} + ''\mathbf{e} + '\mathbf{E}^* + ''\mathbf{E}^*\rangle = |'\mathbf{E}^* + ''\mathbf{E}^*\rangle, \qquad (A1.20)$$

and adding (A1.16) to (A1.17) we deduce, via (A1.5) and (A1.19), that $\mathbf{j}$, $\mathbf{e}$, $\mathbf{J}^*$, and $\mathbf{E}^*$ are solutions to the field equation

$$|\mathbf{j} + \mathbf{J}^*\rangle = \sum_{a=1}^{n} \sigma_a \chi_a |\mathbf{e} + \mathbf{E}^*\rangle, \qquad (A1.21)$$

with $\mathbf{e}, \mathbf{j} \in \mathcal{U}$, $\mathbf{J}^* \in \mathcal{J}'$, and $\mathbf{E}^* \in \mathcal{E}'$. Together with (A1.18), this implies the effective tensor in the Hilbert space $\mathcal{H}'$ is simply just the weighted average of $'\sigma^*$ and $''\sigma^*$, given by (A1.1). Thus the weighted average of two Ω-functions is an Ω-function.

This convexity property of Ω-functions enables us to define classes of extremal Ω-functions: any Ω-function that cannot be expressed as a weighted arithmetic average of Ω-functions is denoted as arithmetic extremal, and their inverses are denoted as harmonic extremal. Clearly an arbitrary Ω-function can be expressed either as a weighted arithmetic average of arithmetic extremal Ω-functions or as a weighted harmonic average of harmonic extremal Ω-functions. Presumably the problem of finding all arithmetic (or harmonic) extremal Ω-functions is related to the currently unsolved problem of finding all the extremal measures of analytic functions [55].

Appendix 2: Generating Ω-Functions by Renormalized Single-Variable Rescaling

To establish that $^\dagger\sigma^*(\sigma_1, \sigma_2, \ldots, \sigma_n)$, defined by (3.19) and (3.20), is indeed an Ω-function, consider the Hilbert space $\mathcal{H}$ and for any field $\mathbf{P} \in \mathcal{H}$ let $\psi^+(\mathbf{P})$ and $\psi^-(\mathbf{P})$ denote the fields obtained via the linear transformations

$$\begin{aligned} \psi^+(\mathbf{P}) &\equiv (I - \chi_1)\mathbf{P} + \lambda^{1/2}\chi_1\mathbf{P}, \\ \psi^-(\mathbf{P}) &\equiv (I - \chi_1)\mathbf{P} + \lambda^{-1/2}\chi_1\mathbf{P}. \end{aligned} \qquad (A2.1)$$

This definition ensures that

$$\langle \psi^+(\mathbf{P})|\psi^-(\mathbf{P}')\rangle = \langle \mathbf{P}|\mathbf{P}'\rangle, \qquad (A2.2)$$

for all $\mathbf{P}, \mathbf{P}' \in \mathcal{H}$. Next define

$$^\dagger\mathcal{U} \equiv [\psi^+(\mathcal{E} \oplus \mathcal{U})] \cap [\psi^-(\mathcal{J} \oplus \mathcal{U})], \qquad (A2.3)$$

and let $^\dagger\mathcal{E}$ and $^\dagger\mathcal{J}$ denote the orthogonal complements of $^\dagger\mathcal{U}$ in the subspaces $\psi^+(\mathcal{E} \oplus \mathcal{U})$ and $\psi^-(\mathcal{J} \oplus \mathcal{U})$ respectively. We leave the subspaces $\mathcal{P}_a$, $a = 1, 2, \ldots, n$, unchanged. Now if the field equation

$$|\mathbf{j} + \mathbf{J}^*(\mathbf{j})\rangle = \left(\lambda\sigma_1\chi_1 + \sum_{a=2}^{n} \sigma_a\chi_a\right)|\mathbf{e} + \mathbf{E}^*(\mathbf{e})\rangle \qquad (A2.4)$$

is satisfied for some $\mathbf{E}^* \in \mathscr{E}$, $J^* \in \mathscr{J}$, and $\mathbf{e}$, $\mathbf{j} \in \mathscr{U}$, then (A2.1) implies that the field equation

$$|^\dagger\mathbf{j} + {}^\dagger\mathbf{J}^*\rangle = \sum_{a=1}^{n} \sigma_a \chi_a |^\dagger\mathbf{e} + {}^\dagger\mathbf{E}^*\rangle \tag{A2.5}$$

has the solution

$$\begin{aligned}
{}^\dagger\mathbf{j} + {}^\dagger\mathbf{J}^* &= \psi^-(\mathbf{j} + \mathbf{J}^*) \in {}^\dagger\mathscr{U} \oplus {}^\dagger\mathscr{J}, \\
{}^\dagger\mathbf{e} + {}^\dagger\mathbf{E}^* &= \psi^+(\mathbf{e} + \mathbf{E}^*) \in {}^\dagger\mathscr{U} \oplus {}^\dagger\mathscr{E},
\end{aligned} \tag{A2.6}$$

from which the components ${}^\dagger\mathbf{e}$, ${}^\dagger\mathbf{j} \in {}^\dagger\mathscr{U}$, ${}^\dagger\mathbf{E}^* \in {}^\dagger\mathscr{E}$, and ${}^\dagger\mathbf{J}^* \in {}^\dagger\mathscr{J}$ can be resolved by projecting onto ${}^\dagger\mathscr{U}$, ${}^\dagger\mathscr{E}$, and ${}^\dagger\mathscr{J}$. In particular it follows that

$$\psi^-(\mathbf{j} + \mathbf{J}^*(\mathbf{j})) = \psi^+(\mathbf{e} + \mathbf{E}^*(\mathbf{e})) \in {}^\dagger\mathscr{U} \quad \text{when} \quad \sigma_a = 1, \quad \forall a. \tag{A2.7}$$

Conversely, any field in ${}^\dagger\mathscr{U}$ generates a solution of (A2.4) when the conductivities σ_a are all equal. Thus given any two sets of d fields $\mathbf{e}_\ell, \mathbf{j}_\ell, \ell = 1, 2, \ldots, d$, each spanning $\mathscr{U}$ and satisfying

$$\mathbf{j}_\ell = {}^\dagger\mathcal{N}\mathbf{e}_\ell, \quad \forall\ell, \tag{A2.8}$$

we can take the fields

$$\mathbf{a}_\ell \equiv \psi^-(\mathbf{j}_\ell + \mathbf{J}^*(\mathbf{j}_\ell)) = \psi^+(\mathbf{e}_\ell + \mathbf{E}^*(\mathbf{e}_\ell)) \quad \text{at} \quad \sigma_a = 1 \quad \forall a \tag{A2.9}$$

as a basis set for ${}^\dagger\mathscr{U}$. From (A2.2) and (A2.8) we have

$$\langle\mathbf{a}_\ell|\mathbf{a}_k\rangle = \langle\mathbf{j}_\ell|\mathbf{e}_k\rangle = \langle{}^\dagger\mathcal{N}\mathbf{e}_\ell|\mathbf{e}_k\rangle, \tag{A2.10}$$

and so to obtain an orthonormal basis set for ${}^\dagger\mathscr{U}$ let us select

$$\mathbf{e}_\ell = {}^\dagger\hat{\mathcal{N}}\mathbf{x}_\ell. \tag{A2.11}$$

None of these uniform fields $\mathbf{e}_\ell$ are zero and consequently the orthogonality of ${}^\dagger\mathscr{U}$ to the subspaces ${}^\dagger\mathscr{E}$ and ${}^\dagger\mathscr{J}$ implies, via (A2.2) and (A2.9), that

$${}^\dagger\mathscr{E} = \psi^+(\mathscr{E}), \qquad {}^\dagger\mathscr{J} = \psi^-(\mathscr{J}), \tag{A2.12}$$

which with (A2.2) establishes the orthogonality of ${}^\dagger\mathscr{E}$ to ${}^\dagger\mathscr{J}$.

Now consider the solutions (A2.6) of (A2.5) for any set of conductivities σ_a, $a = 1, 2, \ldots, n$, that lie in one half of the complex plane. From (A2.6), (A2.9), and (A2.2) we deduce

$$\langle\mathbf{a}_\ell|^\dagger\mathbf{j}\rangle = \langle\mathbf{a}_\ell|^\dagger\mathbf{j} + \mathbf{J}\rangle = \langle\mathbf{e}_\ell|\mathbf{j}\rangle. \tag{A2.13}$$

Substituting (1.1), (3.19), and (A2.11) in this expression gives

$$\langle\mathbf{a}_\ell|^\dagger\mathbf{j}\rangle = \sum_{k=1}^{d} \langle\mathbf{x}_\ell|^\dagger\sigma^*|\mathbf{x}_k\rangle\langle\mathbf{x}_k|^\dagger\hat{\mathcal{N}}|\mathbf{e}\rangle, \tag{A2.14}$$

where (3.20) defines ${}^\dagger\sigma^*$. Similarly, from (A2.2), (A2.6), and (A2.11), we have

$$\langle\mathbf{a}_k|^\dagger\mathbf{e}\rangle = \langle\mathbf{x}_k|^\dagger\hat{\mathcal{N}}|\mathbf{e}\rangle, \tag{A2.15}$$

which in conjunction with (A2.14) implies that ${}^\dagger\sigma^*$ is the effective conductivity matrix associated with the Hilbert space $\mathscr{H} = {}^\dagger\mathscr{U} \oplus {}^\dagger\mathscr{E} \oplus {}^\dagger\mathscr{J}$. Thus an Ω-function

remains an Ω-function under the renormalized single variable rescaling defined by (3.20).

Appendix 3: Substituting a Scalar Ω-Function in a Tensor Ω-Function to Produce a New Ω-Function

Here we prove the $(m+n-1)$-variable function $\sigma^*(\sigma_1, \sigma_2, ..., \sigma_{m+n-1})$ defined by (3.21) is an Ω-function for all n-variable tensor Ω-functions $'\sigma^*('\sigma_1, '\sigma_2, ..., '\sigma_n)$ and for all m-variable scalar Ω-functions $''\sigma^*(''\sigma_1, ''\sigma_2, ..., ''\sigma_m)$. To do this, we adopt the notation of Appendix 1, letting $'\mathscr{H}$ and $''\mathscr{H}$ denote the two Hilbert spaces associated with the Ω-functions $'\sigma^*$ and $''\sigma^*$: all elementary vectors, projection operators and subspaces associated with $'\mathscr{H}$ and $''\mathscr{H}$ are denoted by a single inverted comma and by a pair of inverted commas, respectively. Since the Ω-function $''\sigma^*$ is a scalar Ω-function, the one-dimensional subspace $''\mathscr{U}$ is spanned by a single vector $''\mathbf{x}$.

By analogy with what happens when a composite is substituted as one of the components in another composite, let us introduce the component spaces

$$\mathscr{P}_a' \equiv '\mathscr{P}_1 \otimes ''\mathscr{P}_a \qquad \text{for} \quad 1 \le a \le m$$
$$\equiv '\mathscr{P}_{a+1-m} \otimes ''\mathscr{U} \quad \text{for} \quad m+1 \le a \le n+m-1 \tag{A3.1}$$

labelled by the component index $a = 1, 2, ..., n+m-1$, the three alternative spaces

$$\mathscr{U} \equiv '\mathscr{U} \otimes ''\mathscr{U}, \quad \mathscr{E}' \equiv ('\mathscr{E} \otimes ''\mathscr{U}) \oplus ('\mathscr{P}_1 \otimes ''\mathscr{E}), \quad \mathscr{J}' \equiv ('\mathscr{J} \otimes ''\mathscr{U}) \oplus ('\mathscr{P}_1 \otimes ''\mathscr{J}), \tag{A3.2}$$

and the Hilbert space

$$\mathscr{H}' \equiv \mathscr{U} \oplus \mathscr{E}' \oplus \mathscr{J}' = \mathscr{P}_1' \oplus \mathscr{P}_2' \oplus ... \oplus \mathscr{P}_{m+n-1}', \tag{A3.3}$$

spanned by these spaces. These definitions and the commutability,

$$'A''B = ''B'A, \tag{A3.4}$$

of any operators $'A$ and $''B$ associated with $'\mathscr{H}$ and $''\mathscr{H}$ imply

$$\Gamma_0 \equiv '\Gamma_0 ''\Gamma_0, \quad \Gamma_1 = '\Gamma_1 ''\Gamma_0 + '\chi_1 ''\Gamma_1, \quad \Gamma_2 \equiv '\Gamma_2 ''\Gamma_0 + '\chi_1 ''\Gamma_2, \tag{A3.5}$$

and

$$\chi_a \equiv '\chi_1 ''\chi_a \qquad \text{for} \quad 1 \le a \le m$$
$$\equiv '\chi_{a+1-m} ''\Gamma_0 \quad \text{for} \quad m+1 \le a \le n+m-1, \tag{A3.6}$$

act as projection operators onto the subspaces $\mathscr{U}$, $\mathscr{E}'$, $\mathscr{J}'$, and $\mathscr{P}_a'$ satisfying

$$\Gamma_i \Gamma_j = \delta_{ij} \Gamma_i, \quad \chi_a \chi_b = \delta_{ab} \chi_a. \tag{A3.7}$$

Now suppose the field equations

$$|''\mathbf{j} + '\mathbf{J}^*\rangle = \sum_{a=1}^{n} '\sigma_a '\chi_a |'\mathbf{e} + '\mathbf{E}^*\rangle,$$
$$|''\mathbf{j} + ''\mathbf{J}^*\rangle = \sum_{a=1}^{m} ''\sigma_a ''\chi_a |''\mathbf{e} + ''\mathbf{E}^*\rangle, \tag{A3.8}$$

are solved for the fields $'\mathbf{E}^* \in '\mathscr{E}$, $'\mathbf{J}^* \in '\mathscr{J}$, $''\mathbf{E}^* \in ''\mathscr{E}$, and $''\mathbf{J}^* \in ''\mathscr{J}$ for any $'\mathbf{j} = '\sigma^*'\mathbf{e} \in '\mathscr{U}$ and $''\mathbf{j} = ''\sigma^*''\mathbf{e} \in ''\mathscr{U}$, and let us look for solutions of the field equation

$$|\mathbf{j} + \mathbf{J}^*\rangle = \sum_{a=1}^{n+m-1} \sigma_a \chi_a |\mathbf{e} + \mathbf{E}^*\rangle, \tag{A3.9}$$

where $\mathbf{j} \in \mathscr{U}$, $\mathbf{J}^* \in \mathscr{J}'$ and the fields $\mathbf{e} \in \mathscr{U}$, $\mathbf{E}^* \in \mathscr{E}'$ have the form

$$|\mathbf{e}\rangle = |'\mathbf{e}, ''\mathbf{e}\rangle,$$
$$|\mathbf{E}^*\rangle = |'\mathbf{E}^*, ''\mathbf{e}\rangle + '\chi_1|'\mathbf{e} + '\mathbf{E}^*, ''\mathbf{E}^*\rangle, \tag{A3.10}$$

and the component conductivities are given by

$$\sigma_a = ''\sigma_a \qquad \text{for} \quad 1 \leqq a \leqq m$$
$$= '\sigma_{a+1-m} \quad \text{for} \quad m+1 \leqq a \leqq n+m-1. \tag{A3.11}$$

From (A3.6) and the above equations we have

$$\sum_{a=1}^{n+m-1} \sigma_a \chi_a |\mathbf{e} + \mathbf{E}^*\rangle = |'\mathbf{j} + '\mathbf{J}^*, ''\mathbf{e}\rangle + '\chi_1|'\mathbf{e} + '\mathbf{E}^*, ''\mathbf{J}^*\rangle + (''\sigma^* - '\sigma_1)|'\mathbf{e} + '\mathbf{E}^*, ''\mathbf{j}\rangle, \tag{A3.12}$$

and from (A3.2) this represents a current field $\mathbf{j} + \mathbf{J}^* \in \mathscr{U} \oplus \mathscr{J}'$ if and only if

$$'\sigma_1 = ''\sigma^*, \tag{A3.13}$$

in which case (A3.10) is the solution of the field equation (A3.9) and we have

$$|\mathbf{j}\rangle = \Gamma_0 \sum_{a=1}^{n+m-1} \sigma_a \chi_a |\mathbf{e} + \mathbf{E}^*\rangle = |'\mathbf{j}, ''\mathbf{e}\rangle = '\sigma^*|'\mathbf{e}, ''\mathbf{e}\rangle = '\sigma^*|\mathbf{e}\rangle. \tag{A3.14}$$

This in conjunction with (A3.11) and (A3.13) implies that the function $\sigma^*(\sigma_1, \sigma_2, \ldots, \sigma_{n+m-1})$ defined by (3.21) is the effective conductivity function in the Hilbert space $\mathscr{H}'$ defined by (A3.3) and thus represents an $n+m-1$ variable Ω-function.

Appendix 4: Equivalence of Two Variable Ω-Functions and Normalized Σ-Functions

In Sect. 3 it was established that the class of normalized Σ-functions [i.e. those functions satisfying (3.1–3) and (3.6)] included all Ω-functions. The converse is also true for functions of two variables: any two-variable symmetric matrix-valued normalized Σ-function, $\sigma^*(\sigma_1, \sigma_2)$, can be represented as a continued fraction of, say, the form implied by (2.16) and (2.20–23) for a suitable allowable set of geometric parameters. Our proof of this result draws from the work of Bergman [19] and Golden [28, 55] and thus parallels the approach of Nevanlinna [45, 46] for generating a continued fraction expansion of a single variable Stieltjes or Hamburger function.

To develop the continued fraction expansion, given the normalized Σ-function $\sigma^*(\sigma_1, \sigma_2)$, consider the single-variable matrix-valued function

$$F^{(0)}(s_1) \equiv I - \sigma^*/\sigma_2, \quad \text{where} \quad s_1 = \sigma_2/(\sigma_2 - \sigma_1). \tag{A4.1}$$

From (3.2), (3.3), and (3.6) this function is analytic in s_1 except at points on the real line in the interval $[0, 1]$, is real-symmetric [i.e. has the property that $F^{(0)}(\bar{s}_1) = \overline{F^{(0)}(s_1)}$, where the bar denotes complex conjugation] and satisfies

$$\operatorname{Im} F^{(0)}(s_1) \leq 0 \quad \text{when} \quad \operatorname{Im} s_1 \geq 0, \tag{A4.2}$$

$$F^{(0)}(1) \leq I, \quad F^{(0)}(\infty) = 0. \tag{A4.3}$$

Hence $F^{(0)}(s_1)$ has the integral representation

$$F^{(0)}(s_1) = \int_0^1 \frac{\mu(z)\,dz}{s_1 - z}, \tag{A4.4}$$

where the measure $\mu(z)\,dz$ is real and positive-semidefinite. We define $W_1^{(0)}$ to be the zeroth moment,

$$W_1^{(0)} = \int_0^1 \mu(z)\,dz, \tag{A4.5}$$

which is clearly positive-semidefinite, and from (A4.3) satisfies the bound

$$W_1^{(0)} \leq \int_0^1 \frac{\mu(z)\,dz}{(1-z)} \leq I. \tag{A4.6}$$

This implies the matrix

$$W_2^{(0)} \equiv I - W_1^{(0)} \tag{A4.7}$$

is likewise positive-semidefinite.

Following Bergman [19] and Golden [28, 55] note that the function

$$s_1 F^{(0)}(s_1) = \int_0^1 \frac{s_1 \mu(z)\,dz}{s_1 - z} = W_1^{(0)} + \int_0^1 \frac{z\mu(z)\,dz}{s_1 - z} \tag{A4.8}$$

is real-symmetric, and after subtracting the constant $W_1^{(0)}$ is a function of the same form as $F^{(0)}(s_1)$ but with the new measure $z\mu(z)\,dz$. Therefore we have

$$\operatorname{Im} s_1 F^{(0)}(s_1) \leq 0 \quad \text{when} \quad \operatorname{Im} s_1 \geq 0, \tag{A4.9}$$

which together with (3.11) and (A4.3) implies that the function

$$F^{(1)}(s_1) = I - \hat{W}_1^{(0)} [s_1 F^{(0)}(s_1)]^{-1} \hat{W}_1^{(0)} \tag{A4.10}$$

is similarly real-symmetric, analytic except at points $s_1 \in [0, 1]$ on the real line, and satisfies

$$\operatorname{Im} F^{(1)}(s_1) \leq 0 \quad \text{when} \quad \operatorname{Im} s_1 \geq 0,$$
$$F^{(1)}(1) \leq W_2^{(0)}, \quad F^{(1)}(\infty) = 0. \tag{A4.11}$$

Consequently it has the integral representation

$$F^{(1)}(s_1) = \int_0^1 \frac{\mu^{(1)}(z)\,dz}{s_1 - z}, \tag{A4.12}$$

where the measure $\mu^{(1)}(z)\,dz$ is positive-semidefinite.

By repeating most of this argument the two-variable function

$$\Sigma^{(1)}(\sigma_1, \sigma_2) = \sigma_2 \{\hat{W}_2^{(0)} [s_1 F^{(1)}(s_1)]^{-1} \hat{W}_2^{(0)} - I\} \tag{A4.13}$$

is recognized to be a Σ-function, satisfying (3.2), (3.3), and (3.6). If we choose

$$N^{(1)} = \Sigma^{(1)}(1, 1) \quad (\geqq 0), \tag{A4.14}$$

and define the normalized Σ-function,

$$\Omega^{(1)}(\sigma_1, \sigma_2) = \dot{N}^{(1)} \Sigma^{(1)}(\sigma_1, \sigma_2) \dot{N}^{(1)}, \tag{A4.15}$$

then (A4.1), (A4.10), and (A4.13) imply

$$\sigma^*/\sigma_2 = I + \hat{W}_1^{(0)} \tilde{\Delta}^{+(1)} \hat{W}_1^{(0)}, \tag{A4.16}$$

where

$$\Delta^{+(1)} \equiv \hat{W}_2^{(0)} \tilde{\Pi}^{+(1)} \hat{W}_2^{(0)} - s_1 I, \tag{A4.17}$$

$$\Pi^{+(1)} \equiv I + \hat{N}^{(1)} \Omega^{(1)} \hat{N}^{(1)}/\sigma_2, \tag{A4.18}$$

are defined in accordance with (2.20) and (2.21).

We can now iterate the procedure and obtain a hierarchy of effective tensors $\Omega^{(j)}(\sigma_1, \sigma_2), j = 1, 2, \ldots, \infty$ and allowable $d \times d$ geometric matrices $W_1^{(j)}, W_2^{(j)},$ and $N^{(j)}$. The recursion relations, such as (A4.16–18), between the effective tensors generate a continued fraction expansion for $\sigma^*(\sigma_1, \sigma_2)$ in terms of the allowable geometric parameters. From (2.15) we have

$$Y^{(j-1)} = W_1^{(j)} W_2^{(j)}, \qquad \hat{Y}^{(j+1)} = \hat{W}_1^{(j)} \hat{W}_2^{(j)} \quad \text{for} \quad n = 2, \tag{A4.19}$$

and so the resulting continued fraction is clearly of the form implied by (2.16) and (2.20–23). The equivalence of two-variable Ω-functions and normalized Σ-functions is thus established.

References

1. Milton, G.W.: Multicomponent composites, electrical networks and new types of continued fraction I. Commun. Math. Phys. **111**, 281–327 (1987)
2. Dell'Antonio, G.F., Figari, R., Orlandi, E.: An approach through orthogonal projections to the study of inhomogeneous or random media with linear response. Ann. Inst. Henri Poincaré **44**, 1 (1986)
3. Wiener, O.: Abhandlungen der Mathematisch-Physischen Klasse der Königlichen Sächsischen Gesellschaft der Wissenschaften **32**, 509 (1912)
4. Hashin, Z., Shtrikman, S.: A variational approach to the theory of the effective magnetic permeability of multiphase materials. J. Appl. Phys. **33**, 3125 (1962)
5. Beran, M.J.: Use of the variational approach to determine bounds for the effective permittivity in random media. Nuovo Cimento **38**, 771 (1965)

6. Kröner, E.: Bounds for effective elastic moduli of disordered materials. J. Mech. Phys. Solids **25**, 137 (1977)
7. Phan-Thien, N., Milton, G.W.: New bounds on the effective thermal conductivity of N-phase materials. Proc. R. Soc. Lond A **380**, 333 (1982)
8. Prager, S.: Improved variational bounds on some bulk properties of a two-phase random medium. J. Chem. Phys. **50**, 4305 (1969)
9. Willis, J.R.: Bounds and self-consistent estimates for the overall moduli of anisotropic composites. J. Mech. Phys. Solids **25**, 185 (1977)
10. Murat, F., Tartar, L.: Calcul des variations et homogenisation. In: Les méthodes d'homogénéisation: théorie et applications en physique, Coll. de la Dir. des Etudes et Recherches d'Electricite dé France, pp. 319–370. Paris: Eyrolles 1985
11. Lurie, K.A., Cherkaev, A.V.: Exact estimates of conductivity of composites formed by two isotropically conducting media taken in prescribed proportion. Proc. R. Soc. Edinb. **99**A, 71 (1984)
12. Kohn, R.V., Milton, G.W.: On bounding the effective conductivity of anisotropic composites. In: Homogenization and effective moduli of materials and media. Ericksen, J., Kinderlehrer, D., Kohn, R., Lions, J.L. (eds.). Berlin, Heidelberg, New York: Springer 1986
13. Milton, G.W., Kohn, R.V.: Variational bounds on the effective moduli of anisotropic composites (in preparation)
14. Kohn, R.V., Strang, G.: Optimal design and relaxation of variational problems. Commun. Pure Appl. Math. (to appear)
15. Bendsoe, M.P.: Optimization of plates. Thesis, Math. Inst. Tech. Univ. Denmark, Lyngby, Denmark 1983
16. Bergman, D.J.: The dielectric constant of a composite material – a problem in classical physics. Phys. Rep. C **43**, 377 (1978)
17. Korringa, J.: The influence of pore geometry on the dielectric dispersion of clean sandstones. Geophysics **49**, 1760 (1984)
18. Golden, K., Papanicolaou, G.: Bounds for effective parameters of heterogeneous media by analytic continuation. Commun. Math. Phys. **90**, 473 (1983)
19. Bergman, D.J.: Rigorous bounds for the complex dielectric constant of a two-component composite. Ann. Phys. **138**, 78 (1982)
20. Milton, G.W.: Bounds on the complex permittivity of a two-component composite material. J. Appl. Phys. **52**, 5286 (1981); see also Theoretical studies of the transport properties of inhomogeneous media, unpublished report TP/79/1: University of Sydney 1979
21. Schulgasser, K., Hashin, Z.: Bounds for effective permittivities of lossy dielectric composites. J. Appl. Phys. **47**, 424 (1975)
22. Milton, G.W.: Bounds on the transport and optical properties of a two-component composite. J. Appl. Phys. **52**, 5294 (1981)
23. McPhedran, R.C., Milton, G.W.: Bounds and exact theories for the transport properties of inhomogeneous media. Appl. Phys. A **26**, 207 (1981)
24. McPhedran, R.C., McKenzie, D.R., Milton, G.W.: Extraction of structural information from measured transport properties of composites. Appl. Phys. A **29**, 19 (1982)
25. Gajdardziska-Josifovska, M.: Optical properties and microstructure of cermets. Unpublished M. Sc. thesis: University of Sydney 1986
26. Felderhof, B.U.: Bounds for the complex dielectric constant of a two-phase composite. Physica **126**A, 430 (1984)
27. Milton, G.W., Golden, K.: Thermal conduction in composites. In: Thermal conductivity 18. Ashworth, T., Smith, D.R. (eds.). New York: Plenum Press 1985
28. Golden, K.: Bounds on the complex permittivity of a multicomponent material. J. Mech. Phys. Solids **34**, 333 (1986)
29. Milton, G.W., McPhedran, R.C.: A comparison of two methods for deriving bounds on the effective conductivity of composites. In: Macroscopic properties of disordered media. Burridge, R. et al. (eds.). Lecture Notes in Physics, Vol. 154, p. 183. Berlin, Heidelberg, New York: Springer 1982

30. Keller, J.B.: A theorem on the conductivity of a composite medium. J. Math. Phys. **5**, 548 (1964)

31. Torquato, S., Beasley, J.D.: Effective properties of fibre-reinforced materials. I. Bounds on the effective thermal conductivity of dispersions of fully penetrable cylinders. Int. J. Engng. Sci. **24**, 415 (1986)

32. Stell, G., Joslin, C.: To be published

33. Schulgasser, K.: On a phase interchange relationship for composite materials. J. Math. Phys. **17**, 378 (1976)

34. Korringa, J., LaTorraca, G.A.: Application of the Bergman-Milton theory of bounds to the permittivity of rocks. J. Appl. Phys. **60**, 2966 (1986)

35. Hashin, J.: Analysis of composite materials. J. Appl. Mech. Trans. ASME **50**, 481 (1983)

36. McPhedran, R.C., McKenzie, D.R., Phan-Thien, N.: Transport properties of two-phase composite materials. In: Advances in the mechanics and flow of granular materials. Shahinpoor, M., Wohlbier, R. (eds.). New York: McGraw-Hill 1983

37. Willis, J.R.: Variational and related methods for the overall properties of composite materials. In: Advances in applied mechanics. Yih, C.-S. (ed.) New York: Academic Press **21**, 2–78 (1981)

38. McCoy, J.J.: Macroscopic response of continua with random microstructures. In: Mechanics today, Nemat-Nasser, S. (ed.), pp. 1–40. Oxford, New York: Pergamon Press 1981

39. Christensen, R.M.: Mechanics of composite materials. New York: Wiley 1979

40. Watt, J.P., Davies, G.F., O'Connell, R.J.: The elastic properties of composite materials. Rev. Geophy. Space Phys. **14**, 541 (1976)

41. Hale, D.K.: The physical properties of composite materials. J. Mater. Sci. **11**, 2105 (1976)

42. Beran, M.J.: Statistical continuum theories, pp. 181–256. New York: Interscience 1968

43. Niklasson, G.A., Granquist, C.G.: Optical properties and solar selectivity of coevaporated Co–Al_2O_3 composite films. J. Appl. Phys. **55**, 3382 (1984)

44. Torquato, S., Stell, G.: Macroscopic approach to transport in two-phase random media. CEAS report #352 1980

45. Nevanlinna, R.: Asymptotische Entwickelungen beschrankter Funktionen und das Stielt-jessche Momenten problem. Ann. Acad. Sci. Fenn. A **18**, 1 (1922)

46. Shohat, J.A., Tamarkin, J.D.: The problem of moments. Baltimore: Waverly Press 1943

47. Henrici, P., Pfluger, P.: Truncation error estimates for Stieltjes fractions. Numer. Math. **9**, 129 (1966)

48. Gragg, W.B.: Truncation error bounds for g-fractions. Numer. Math. **11**, 370 (1968)

49. Common, A.K.: Páde approximants and bounds to series of Stieltjes. J. Math. Phys. **9**, 32 (1967)

50. Baker, G.A., Jr.: Best error bounds for Padé approximants to convergent series of Stieltjes. J. Math. Phys. **10**, 814 (1969)

51. Baker, G.A., Jr., Graves-Morris, P.R.: Encyclopedia of mathematics and its applications, Vols. 13 and 14. Rota, G.-C. (ed.). London: Addison-Wesley 1981

52. Jones, W.B., Thron, W.J.: Encyclopedia of mathematics and its applications, Vol. 11. Rota, G.-C. (ed.). London: Addison-Wesley 1980

53. Golden, K., Papanicolaou, G.: Bounds for effective parameters of multicomponent media by analytic continuation. J. Stat. Phys. **40**, 655 (1985)

54. Bergman, D.J., Milton, G.W.: Unpublished

55. Golden, K.: Bounds for effective parameters of multicomponent media by analytic continuation. Ph. D. thesis: New York University 1984

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