Bounds for Effective Parameters of Multicomponent Media by Analytic Continuation

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ABSTRACT

Recently D. Bergman introduced a method for obtaining bounds on the effective dielectric constant of a two-component medium. This method exploits the properties of the effective parameter as an analytic function of the ratio of the component parameters. We give a mathematical formulation of the method and extend it to multicomponent media using techniques of several complex variables. The extension is used to rederive known real bounds and to obtain new complex bounds for multicomponent media.

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1. Introduction

Due to the difficulty of calculating the effective parameter (e.g., dielectric constant, magnetic permeability, or electrical or thermal conductivity) of a heterogeneous medium, there has been much interest in obtaining bounds on these parameters. Wiener [1] gave optimal bounds on the effective parameter of a multicomponent material with fixed volume fractions and real component parameters. For isotropic materials, Hashin and Shtrikman [2] improved Wiener's bounds using variational principles. Recently Bergman [3-10] introduced a method for obtaining bounds on complex effective parameters which does not rely on variational principles. Instead it exploits the properties of the effective parameter as an analytic function of the component parameters. The method of Bergman has been elaborated upon in detail and applied to several problems by Milton [11-16]. A mathematical formulation of it was given by Golden and Papanicolaou in [17]. However, the method has been restricted to two-component materials, where the effective parameter is a function of a single complex variable, the ratio of the component parameters. In this thesis the method is extended to multicomponent media for the first time. In particular, we obtain the analog for several complex variables of the single variable integral representation for the effective parameter given in [17]. The extended representation formula is used to rederive the Wiener and Hashin-Shtrikman bounds for multicomponent media with real parameters and to obtain new complex versions of them. This is facilitated by introducing a new fractional linear transformation of the effective parameter which diagonalizes to second order the perturbation expansion of the effective parameter about a homogeneous medium. In addition, the method for two-component media is reviewed in detail. In the review we give an infinite sequence of optimal bounds which include more and more information about the material, by using successive fractional linear transformations of the effective parameter.

In [17] the integral representation involves a complex kernel, which contains the component parameter information, and a positive measure, which contains the mixture geometry information. For three-component materials the effective parameter is an analytic function of two complex variables. When one of these variables is fixed as a multiple of the other the effective parameter is an analytic function of a single variable. Bergman [3,9] has applied the analytic method for a single variable in this case to obtain the classical Hashin-Shtrikman bounds for real component parameters. However, this approach makes the above mentioned measure depend upon the component parameters as well as the geometry of the composite. The problem in giving a direct extension of the analytic continuation method to multicomponent media has been to find a representation for the effective parameter which indeed separates the component parameters from the geometry. We have done this by exploiting the analyticity properties of the effective parameter as a function of several complex variables.

The multicomponent representation formula is significant for the following reason. Like the two-component case, the effective parameter can be expanded about a homogeneous medium where the component parameters are equal. The information in this perturbation expansion can then be used along with the representation formula to continue the effective parameter beyond nearly homogeneous materials to its full domain of analyticity.

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2. Formulation of the Multicomponent Problem

We assume that the medium under study is an N-component microscopically isotropic dielectric (or conducting) material. Our formulation of the effective parameter problem is the same as in [17] and [18].

Let $(\Omega, \mathcal{F}, P)$ be a probability space and let $\varepsilon_{ij}(x,\omega)$ be strictly stationary random fields on $x \in \mathbb{R}^d$, $\omega \in \Omega$, $i,j = 1,2,\cdots,d$. The $\varepsilon_{ij}(x,\omega)$ represent the dielectric constant at $x \in \mathbb{R}^d$ for the realization $\omega \in \Omega$ of the medium. Strict stationarity means here that the joint distribution of $\varepsilon_{ij}(x_1,\omega)$, $\varepsilon_{ij}(x_2,\omega)$, $\cdots$, $\varepsilon_{ij}(x_n,\omega)$ for any $x_1,x_2,\cdots,x_n \in \mathbb{R}^d$ is the same as that of $\varepsilon_{ij}(x_1+h, \omega)$, $\varepsilon_{ij}(x_2+h, \omega)$, $\cdots$, $\varepsilon_{ij}(x_n+h, \omega)$ for any $h \in \mathbb{R}^d$. In particular, we assume the existence of a translation group τ_x, $x \in \mathbb{R}^d$, which is one to one on Ω and preserves P. With each strictly stationary random field $f(x,\omega)$ we associate a measurable function $f(\omega)$ via

$$f(\tau_{-x}\omega) = f(x,\omega) \quad . \tag{2.1}$$

By stationarity we focus attention at $x = 0$, so that $f(\omega) = f(0,\omega)$.

Let $E^k(x,\omega)$ and $D^k(x,\omega)$ be two stationary random vector fields satisfying

$$D_i^k(x,\omega) = \sum_{j=1}^{d} \varepsilon_{ij}(x,\omega)\, E_j^k(x,\omega) \ , \ i = 1,\cdots,d, \tag{2.2}$$

$$\nabla \cdot D^k(x,\omega) = 0 \tag{2.3}$$

$$\nabla \times E^k(x,\omega) = 0 \tag{2.4}$$

$$\int_\Omega P(d\omega)\, E^k(x,\omega) = e_k, \tag{2.5}$$

where e_k is a unit vector in the k^{th} direction for some $k = 1,2,\cdots, d$. For an oscillating electric field the dielectric constant is complex, with the real part corresponding to the polarizability of the medium and the imaginary part corresponding to its conductivity. We assume that the wavelength of the field is much larger than the scale of the inhomogeneities so that (2.4) may still be assumed to hold.

The effective dielectric constant ε^*_{ik} may now be defined

$$\varepsilon^*_{ik} = \int_\Omega P(d\omega)\, D^k_i(\omega)\ , \quad i = 1,\cdots,d. \tag{2.6}$$

Note that definition (2.6) is an ensemble average in an infinite stationary medium. In [17] we showed that this definition coincides with the more standard one involving a volume average.

3. Existence and Uniqueness of the Electric Field.

The analysis is the same as in [17]. The group of transformations τ_x acting on Ω induces a group of operators on the Hilbert space of complex valued functions $H = L^2(\Omega, \mathcal{F}, P)$ with inner product

$$(f,g) = \int_\Omega P(d\omega)\, f(\omega)\, \overline{g(\omega)}\,, \quad f,g \in H. \tag{3.1}$$

The operators T_x on H are given by

$$(T_x f)(\omega) = f(\tau_{-x}\omega),\ x \in \mathbb{R}^d, \tag{3.2}$$

and form a unitary group since τ_x is measure preserving. This group has closed, densely defined infinitesimal generators in each direction of $\mathbb{R}^d$,

$$L_i = \frac{\partial}{\partial x_i} T_x \Big|_{x=0},\ i = 1,2,\cdots,d. \tag{3.3}$$

The differentiation is defined in the sense of convergence in H for elements of $\mathcal{D}_i$, the domain of L_i. We are of course interested in fields contained in $\mathcal{D} = \bigcap_{i=1}^{d} \mathcal{D}_i$.

The problem (2.2) - (2.5) may now be formulated as follows. Let $\mathcal{H}$ be the Hilbert space

$$\mathcal{H} = \{f_i(\omega) \in H,\ i = 1,2,\cdots,d\ |L_i f_j = L_j f_i \text{ weakly} \text{ and } \int_\Omega P(d\omega)\, f_i(\omega) = 0\}. \tag{3.4}$$

Now the problem becomes to find $G_i^k(\omega) \in \mathcal{H}$ such that

$$\int_\Omega P(d\omega) \sum_{i,j=1}^{d} \varepsilon_{ij}(\omega)(G_j^k(\omega) + \delta_{jk})\overline{f_i}(\omega) = 0, \tag{3.5}$$

for all $f_i \in \mathcal{H}$. When the form associated with (3.5) is coercive, this problem has a unique solution by the Lax-Milgram lemma. Clearly

$$E^k(\omega) = e_k + G^k(\omega)$$

$$D_i^k(\omega) = \sum_{j=1}^{d} \varepsilon_{ij}(\omega)\, E_j^k(\omega) \tag{3.6}$$

is the unique solution of (2.2) - (2.5) via (2.1).

4. Analyticity of the Effective Parameter

We focus our attention on N-component media of the form

$$\varepsilon_{ij}(\omega) = \varepsilon(\omega)\delta_{ij} \tag{4.1}$$

where $\varepsilon(\omega)$ takes N complex values and may be written as

$$\varepsilon(\omega) = \sum_{\ell=1}^{N} \varepsilon_\ell \, \chi_\ell(\omega). \tag{4.2}$$

The indicator function $\chi_\ell(\omega)$ of medium ℓ equals one for all realizations $\omega \in \Omega$ which have medium ℓ at $x = 0$ and equals zero otherwise.

Since (2.2) - (2.6) are linear in $\varepsilon(\omega)$, the effective parameter depends only on the ratios

$$h_i = \frac{\varepsilon_i}{\varepsilon_N}, \quad i = 1,2,\cdots,n, \tag{4.3}$$

where $n = N-1$. We write

$$m_{ik}(h_1,\cdots,h_n) = \frac{\varepsilon^*_{ik}}{\varepsilon_N} = \int_\Omega P(d\omega)\left(\sum_{j=1}^{n} h_j \chi_j(\omega) + \chi_N(\omega)\right) E^k_i(\omega). \tag{4.4}$$

From (4.4) it is clear that m_{ik} has the same domain of analyticity in $\mathbb{C}^n$ as does $E^k_i(\omega)$. The form associated with (3.5) is coercive when there is an $\alpha > 0$ such that

$$\left| \int_\Omega P(d\omega)\left(\sum_{j=1}^{n} h_j \chi_j + \chi_N\right) \sum_{i=1}^{d} |G^k_i|^2 \right| \geq \alpha \int_\Omega P(d\omega) \sum_{i=1}^{d} |G^k_i|^2. \tag{4.5}$$

Setting

$$\lambda_j = \frac{\int_\Omega P(d\omega)\chi_j \sum_{i=1}^{d} |G_i^k|^2}{\int_\Omega P(d\omega) \sum_{i=1}^{d} |G_i^k|^2}, \quad j=1,2,\cdots,N, \tag{4.6}$$

with $0 \leq \lambda_j \leq 1$ and $\sum_{j=1}^{N} \lambda_j = 1$ transforms (4.5) to

$$\left| \sum_{j=1}^{n} h_j\lambda_j + \lambda_N \right| \geq \alpha > 0. \tag{4.7}$$

Consequently there exists a unique solution to (3.5) whenever the convex hull of $\{1,h_1,h_2,\cdots,h_n\}$ does not contain the origin in $\mathbb{C}$.

Furthermore, we show that when (4.7) is true, $E_i^k(\omega)$ is analytic in $h_1,\cdots,h_n$. We need only show that $G_i^k(\omega)$ is analytic in $h_1,h_2,\cdots,h_n$. Using (4.1) we can rewrite (3.5) as

$$\int_\Omega P(d\omega) \left(\sum_{j=1}^{n} h_j\chi_j + \chi_N \right) \sum_i G_i^k \bar{f}_i = - \int_\Omega P(d\omega) \left(\sum_{j=1}^{n} h_j\chi_j + \chi_N \right) \bar{f}_k, \tag{4.8}$$

for all $f_i \in \mathcal{H}$. The functional on the right is analytic in $h_1,h_2, \cdots,h_n$, so that the functional involving G_i^k on the left is also. Clearly then the functional

$$\int_\Omega P(d\omega) \sum_i G_i^k \bar{f}_i \quad , \forall f_i \in \mathcal{H}, \tag{4.9}$$

is also analytic in $h_1,h_2,\cdots,h_n$. This means that G_i^k is weakly analytic as a member of $\mathcal{H}$. Since G_i^k is a member of a Hilbert space (a Fréchet space would work), G_i^k is strongly analytic in $h_1,\cdots,h_n$

where the analyticity is defined in the topology of $\mathscr{H}$. Thus, we have that m_{ik} is analytic in the following region of $\mathbb{C}^n$,

$$\mathscr{A} = \{(h_1,\cdots,h_n)\text{: the convex hull of } \{1,h_1,\cdots,h_n\} \text{ in } \mathbb{C} \text{ does not contain the origin in } \mathbb{C}\}. \tag{4.10}$$

In view of (3.5) and (4.1) we can write ε^*_{ik} in the form

$$\varepsilon^*_{ik} = \int_\Omega P(d\omega) \sum_{j=1}^{d} \varepsilon(\omega)\, E^k_j(\omega) \overline{E^i_j(\omega)} \quad . \tag{4.11}$$

This symmetric formula can be verified by substituting $E^i_j = \delta_{ij} + G^i_j$ and then using (3.5) to obtain (2.6) under (4.1). Now let $\tilde{U}^n = \{\text{Im } h_1 > 0\} \times \{\text{Im } h_2 > 0\} \times . \ . \ . \times \{\text{Im } h_n > 0\}$. From the above condition for analyticity we have that $m_{ik}(h_1,\cdots,h_n)$ is analytic in $\tilde{U}^n$. From (4.11) we see that the diagonals m_{kk} map $\tilde{U}^n$ into $\text{Im } m_{kk} > 0$ with the property that

$$m_{kk}(\bar{h}_1,\bar{h}_2,\cdots,\bar{h}_n) = \overline{m_{kk}(h_1,h_2,\cdots,h_n)} \ . \tag{4.12}$$

We will exploit these properties of m_{kk} to obtain a representation formula for the effective parameter analogous to that given in [17].

5. The Operator Representation for the Effective Parameter

For simplicity we will now restrict the discussion to three-component materials with parameters h_1 and h_2. The generalization to more components will be clear. Before we derive the previously mentioned representation formula, it is useful to analyze the analogue for three-component materials of the spectral argument given in [17].

We interpret the standard differential operators in $\mathbb{R}^d$ in terms of the infinitesimal generators in (3.3),

$$\Delta = \sum_{i=1}^{d} L_i^2 \tag{5.1}$$

$$\nabla = (L_1, L_2, \cdots, L_d). \tag{5.2}$$

Now let

$$\Gamma = \nabla(-\Delta)^{-1}\nabla\cdot, \tag{5.3}$$

and in coordinates

$$\Gamma_{ik} = L_i(-\Delta)^{-1}L_k. \tag{5.4}$$

The operators Γ_{ik} are well defined and bounded in $L^2(\Omega,\mathcal{F},P)$ and have norm less than or equal to one, as in the usual case $L_i = \partial/\partial x_i$.

It is convenient to introduce the function

$$F_{ik}(s_1,s_2) = \delta_{ik} - m_{ik}(h_1,h_2) = \int_\Omega P(d\omega)\left(\frac{1}{s_1}\chi_1 + \frac{1}{s_2}\chi_2\right) E_i^k \tag{5.5}$$

with the variables

$$s_1 = \frac{1}{1-h_1}, \quad s_2 = \frac{1}{1-h_2}. \tag{5.6}$$

Understood to hold in the weak form (3.5), the divergence equation (2.3) may be written formally as

$$\sum_{i=1}^{d} L_i \, [(h_1\chi_1 + h_2\chi_2 + \chi_3)E_i^k] = 0. \tag{5.7}$$

Using the operator Γ equation (5.7) can be solved for the electric field

$$E^k(\omega) = (I + \frac{1}{s_1}\Gamma\chi_1 + \frac{1}{s_2}\Gamma\chi_2)^{-1}e_k, \tag{5.8}$$

where I is the identity operator. Substitution into (5.5) yields

$$F_{ik}(s_1,s_2) = \int_\Omega P(d\omega)\,[\frac{\frac{1}{s_1}\chi_1 + \frac{1}{s_2}\chi_2}{I + \frac{1}{s_1}\Gamma\chi_1 + \frac{1}{s_2}\Gamma\chi_2}\; e_k] \cdot e_i, \tag{5.9}$$

where the ratio in (5.9) is understood as in (5.8). If we let $U^2 = \{\mathrm{Im}\, s_1 > 0\} \times \{\mathrm{Im}\, s_2 > 0\}$, then the diagonals $F_{kk}(s_1,s_2)$ map U^2 into $\mathrm{Im}\,(-F_{kk}) > 0$.

For the two-component case, which is obtained from (5.9) in the limit $s_2 \to \infty$, the representation formula given in [17] can be obtained through spectral analysis of $\Gamma\chi_1$. In the three-component case the operators $\Gamma\chi_1$ and $\Gamma\chi_2$ do not commute. For this reason the spectral argument used to obtain the integral formula in [17] does not immediately extend to three components.

6. Bounds for Two-Component Media

A. The Integral Representation

Let

$$h = \frac{\varepsilon_1}{\varepsilon_2},\ s = \frac{1}{1-h},\ F_{ik} = \delta_{ik} - m_{ik}(h). \tag{6.1}$$

The considerations of section 4 tell us that for two-component media $m_{ik}(h)$ is analytic off $(-\infty,0]$, the negative real axis including zero. Equivalently, $F_{ik}(s)$ is analytic off $[0,1]$. In [17] we proved that there exist finite Borel measures $\mu_{ik}(dz)$ defined on $0 \leq z \leq 1$ such that the diagonals $\mu_{kk}(dz)$ are positive and

$$F_{ik}(s) = \int_0^1 \frac{\mu_{ik}(dz)}{s-z},\ i,k = 1,2,\cdots,d \tag{6.2}$$

for all complex s outside $[0,1]$.

The first proof we gave depends on the operator representation

$$F_{ik}(s) = \int_\Omega P(d\omega)\left[\frac{\chi_1}{s+\Gamma\chi_1} e_k\right]\cdot e_i. \tag{6.3}$$

In the Hilbert space

$$\mathcal{H} = \{f_i(\omega) \in L^2(\Omega,\mathcal{F},P)\} \tag{6.4}$$

under the inner product

$$\langle f,g\rangle = \int_\Omega P(d\omega)\,\chi_1(\omega)\sum_{i=1}^{d} f_i(\omega)\overline{g_i(\omega)} \quad , \tag{6.5}$$

the operator $\Gamma\chi_1$ is self adjoint and has norm less than or equal to one. An application of the spectral theorem yields the family of projections Q(dz) associated with $\Gamma\chi_1$ so that (6.3) may be written as

$$F_{ik}(s) = \int_{-1}^{1} \frac{\langle Q(dz)e_k, e_i\rangle}{s+z} \, . \tag{6.6}$$

Using the fact that $F_{ik}(s)$ is analytic off [0,1] and then renaming Q(dz) gives (6.2) with

$$\begin{aligned}\mu_{ik}(dz) &= \int_\Omega P(d\omega)\chi_1(\omega)\, Q(dz)e_k\cdot e_i \\ &= \langle Q(dz)e_k, e_i\rangle. \end{aligned} \tag{6.7}$$

The second proof exploits the fact that $-F_{kk}(s)$ has positive imaginary part when Im $s > 0$ and is analytic at $s = \infty$. In particular, there is a constant M such that

$$|sF_{kk}(\sqrt{-1}\,s)| \leq M, \qquad s > 0. \tag{6.8}$$

Then a general representation theorem in function theory [19], combined with the fact that $F_{kk}(s)$ is analytic off [0,1] gives (6.2) for the diagonals $i = k$.

B. The Perturbation Expansion and its Analytic Continuation

For $|s| > 1$ we can expand (6.3) about a homogeneous medium ($s = \infty$ or $h = 1$),

$$F_{ik}(s) = \int_{\Omega} P(d\omega)\left[\left(\frac{\chi_1}{s} - \frac{\chi_1\Gamma\chi_1}{s^2} + \frac{\chi_1(\Gamma\chi_1)^2}{s^3} - \cdots\right)e_k\right]\cdot e_i. \tag{6.9}$$

Doing the same to (6.2) gives

$$F_{ik}(s) = \frac{\mu_{ik}^{(0)}}{s} + \frac{\mu_{ik}^{(1)}}{s^2} + \frac{\mu_{ik}^{(2)}}{s^3} + \cdots, \tag{6.10}$$

where

$$\mu_{ik}^{(n)} = \int_0^1 z^n\, \mu_{ik}(dz). \tag{6.11}$$

Equating (6.9) to (6.10) gives

$$\mu_{ik}^{(n)} = (-1)^n \int_{\Omega} P(d\omega)\left[\chi_1(\Gamma\chi_1)^n e_k\right] \cdot e_i. \tag{6.12}$$

When $i = k$ the moments of the positive measures are determined by (6.12). Since positive finite measures on compact sets are uniquely determined by their moments, for $i = k$ (6.2) provides the analytic continuation of (6.9) to the full complex s-plane excluding [0,1]. When $i \neq k$, μ_{ik} is a signed measure of mass 0.

Now focus attention on one diagonal coefficient $m_{kk}(h)$ and call it m(h) with

$$F(s) = 1 - m(h) = \int_0^1 \frac{\mu(dz)}{s - z}, \quad s \notin [0,1]. \tag{6.13}$$

From (6.12) we see that

$$\mu^{(0)} = p_1, \tag{6.14}$$

where p_1 is the volume fraction of medium 1. For $\mu^{(1)}$ we have

$$\mu^{(1)} = -\int_\Omega P(d\omega)\, \chi_1(\omega)(\Gamma_{kk}\chi_1)(\omega). \tag{6.15}$$

To evaluate the integral in (6.15), note that Γ_{kk} is bounded on $L^2(\Omega,\mathcal{F},P)$. Then

$$A_{kk} = \frac{\partial}{\partial x_k}(-\Delta)^{-1}\frac{\partial}{\partial x_k}\ ,\ k = 1,2,\cdots,d \tag{6.16}$$

is bounded on $L^2(\mathbb{R}^d)$, so that it is bounded on square integrable stationary random fields.

We may write (6.15) in the form

$$\mu^{(1)} = -\int_\Omega P(d\omega)\chi_1(x,\omega)\frac{\partial^2}{\partial x_k^2}(-\Delta)^{-1}(\chi_1(x,\omega) - p_1)$$

$$= \int_{\mathbb{R}^d} G_{kk}(y)\, R(y)\, dy \quad , \tag{6.17}$$

where $G_{kk}(y)$ is the kernel of the singular integral operator A_{kk} and $R(y)$ is the correlation function

$$R(y) = \int_\Omega P(d\omega)\, \chi_1(x+y,\omega)(\chi_1(x,\omega) - p_1). \tag{6.18}$$

For statistically isotropic media $R(y)$ depends only on $|y|$, so that

$$\mu^{(1)} = \frac{R(0)}{d} = \frac{p_1 p_2}{d}, \qquad (6.19)$$

where $p_2 = 1 - p_1$ is the volume fraction of medium 2.

The higher moments $\mu^{(n)}$, $n \geq 2$ depend on (n+1)-point correlation functions and cannot be calculated in general. However for statistically isotropic materials, the following relationships among the moments are implied by

$$m(h)m(1/h) \geq 1, \qquad (6.20)$$

which holds for $d \geq 3$ and $h \geq 1$. In dimension $d = 2$ the inequality becomes an equality. Keller [20] first proved the result in $d = 2$ and Shulgasser [21] proved (6.20). In [22] the relationship is proved in full generality in a simple manner.

In terms of F(s), (6.20) becomes

$$F(s)F(1-s) \geq F(s) + F(1-s). \qquad (6.21)$$

Let

$$F = \int_0^1 \frac{\mu(dz)}{s - z}, \quad Q = \int_0^1 \frac{\mu(dz)}{1-s-z}. \qquad (6.22)$$

Expanding both expressions in (6.22) about $s = \frac{1}{2}$ gives

$$F = \frac{1}{(s - 1/2)} \int_0^1 \left(1 + \frac{(z - 1/2)}{(s - 1/2)} + \frac{(z - 1/2)^2}{(s - 1/2)^2} + \cdots\right) \mu(dz) \qquad (6.23)$$

$$Q = \frac{-1}{(s - 1/2)} \int_0^1 \left(1 - \frac{(z - 1/2)}{(s - 1/2)} + \frac{(z - 1/2)^2}{(s - 1/2)^2} - \cdots\right) \mu(dz). \tag{6.24}$$

Now we have

$$F + Q = \frac{2a_2}{(s - 1/2)^2} + \frac{2a_4}{(s - 1/2)^4} + \frac{2a_6}{(s - 1/2)^6} + \cdots \tag{6.25}$$

$$FQ = \frac{b_2}{(s - 1/2)^2} + \frac{b_4}{(s - 1/2)^4} + \frac{b_6}{(s - 1/2)^6} + \cdots \tag{6.26}$$

where

$$a_{n+1} = \sum_{k=0}^{n} \binom{n}{k} \left(\frac{-1}{2}\right)^{n-k} \mu^{(k)}, \quad n \geq 0 \tag{6.27}$$

$$b_n = (-1)^{n/2} a^2_{n/2} + \sum_{k=1}^{n/2-1} 2(-1)^k a_k a_{n-k}, \quad n \geq 2 \text{ even}, \; a_0 = 0. \tag{6.28}$$

The interchange inequality (6.20) then imposes the following constraints on the moments

$$b_n \geq 2a_n, \quad n \geq 2 \text{ even}. \tag{6.29}$$

In dimension d = 2 the inequality becomes an equality, which for n = 2 gives

$$\mu^{(1)} = \frac{\mu^{(0)}}{2}(1 - \mu^{(0)}) \qquad (6.30)$$

which is just (6.19). For n = 3,

$$\mu^{(3)} = \frac{\mu^{(2)}}{2}(3 - 2\mu^{(0)}) - \frac{\mu^{(1)}}{2}(1 - \mu^{(0)} - \mu^{(1)}). \qquad (6.31)$$

Here the interchange equality determines the odd moments of μ in terms of the lower order even moments.

In the case of microscopically isotropic yet macroscopically anisotropic materials, the Keller equality for d = 2 [22] becomes

$$m_{11}(h)\, m_{22}(\frac{1}{h}) = 1 \ , \qquad (6.32)$$

where

$$1 - m_{11}(h) = F_{11}(s) = \int_0^1 \frac{\mu_{11}(dz)}{s - z}$$

$$(6.33)$$

$$1 - m_{22}(h) = F_{22}(s) = \int_0^1 \frac{\mu_{22}(dz)}{s - z} \ .$$

Equation (6.32) can be written as

$$F_{11}(s) + F_{22}(1-s) = F_{11}(s)F_{22}(1-s). \qquad (6.34)$$

Analogous to (6.23) and (6.24),

$$F_{11} = \frac{1}{(s - 1/2)} \int_0^1 (1 + (\frac{z - 1/2}{s - 1/2}) + (\frac{z - 1/2}{s - 1/2})^2 + \cdots) \mu_{11}(dz) \qquad (6.35)$$

$$F_{22} = \frac{-1}{(s - 1/2)} \int_0^1 (1 - (\frac{z - 1/2}{s - 1/2}) + (\frac{z - 1/2}{s - 1/2})^2 - \cdots) \mu_{22}(dz) , \qquad (6.36)$$

so that

$$F_{11} + F_{22} = \frac{\mu_{11}^{(0)} - \mu_{22}^{(0)}}{(s - 1/2)} + \frac{\mu_{11}^{(1)} - \frac{1}{2}\mu_{11}^{(0)} + \mu_{22}^{(1)} - \frac{1}{2}\mu_{22}^{(0)}}{(s - 1/2)^2}$$

$$+ \frac{\mu_{11}^{(2)} - \mu_{11}^{(1)} + \frac{1}{4}\mu_{11}^{(0)} - (\mu_{22}^{(2)} - \mu_{22}^{(1)} + \frac{1}{4}\mu_{22}^{(0)})}{(s - 1/2)^3} + \cdots \qquad (6.37)$$

and

$$F_{11}F_{22} = \frac{-\mu_{11}^{(0)}\mu_{22}^{(0)}}{(s - 1/2)^2} + \frac{\mu_{11}^{(0)}(\mu_{22}^{(1)} - \frac{1}{2}\mu_{22}^{(0)}) - \mu_{22}^{(0)}(\mu_{11}^{(1)} - \frac{1}{2}\mu_{11}^{(0)})}{(s - 1/2)^3} + \cdots \quad . \qquad (6.38)$$

Due to (6.14) and the equality of (6.37) and (6.38) we have to third order

$$\mu_{11}^{(0)} = \mu_{22}^{(0)} = p_1 \qquad (6.39)$$

$$\mu_{11}^{(1)} + \mu_{22}^{(1)} = p_1 p_2 \qquad (6.40)$$

$$\mu_{22}^{(2)} - \mu_{11}^{(2)} = p_2(\mu_{22}^{(1)} - \mu_{11}^{(1)}). \qquad (6.41)$$

C. Incorporation of Constraints on the Measure

As in (6.13) we focus on a diagonal coefficient in a macroscopically isotropic medium with

$$F(s) = 1 - m(h) = \int_0^1 \frac{\mu(dz)}{s - z}, \quad s \notin [0,1]. \tag{6.42}$$

The measure μ belongs to the set M of positive finite Borel measures on [0,1]. For s fixed outside [0,1], F is a linear mapping from M into $\mathbb{C}$. Let

$$M(N) = M(\mu^{(0)},\mu^{(1)},\cdots,\mu^{(N)}) = \{\mu \in M \,|\, \int_0^1 z^n \mu(dz) = \mu^{(n)}, n=0,\cdots,N\}, \tag{6.43}$$

provided that $\mu^{(0)},\mu^{(1)},\cdots,\mu^{(N)}$ form a positive definite sequence [23] so that they can represent the moments of a measure. If the first N moments $\mu^{(0)},\mu^{(1)},\cdots,\mu^{(N)}$ of μ are known via (6.9), then F for fixed s is a linear mapping of M(N) into $\mathbb{C}$. In the weak* topology over the continuous functions on [0,1], M(N) is a compact convex subset of M. The image $\Lambda(N) = \Lambda(\mu^{(0)},\cdots,\mu^{(N)})$ of M(N) under F is a compact convex subset of $\mathbb{C}$. Thus one way of characterizing $\Lambda(N)$ is to characterize the extreme points of M(N).

The extreme points of $M(\mu^{(0)})$ are the one-point measures $\mu^{(0)}\delta_y(dz)$ where $\mu^{(0)} \geq 0$ and $0 \leq y \leq 1$. The extreme points of M(N) are the (N+1) - point measures [24]

$$\mu(dz) = \sum_{k=1}^{N+1} \alpha_k \, \delta_{z_k}(dz), \tag{6.44}$$

where

$$\alpha_k \geq 0,\ \ 0 \leq z_1 \leq \cdots \leq z_{N+1} \leq 1,\ \sum_{k=1}^{N+1} \alpha_k z_k^n = \mu^{(n)},\ \ n = 0,1,\cdots,N. \qquad (6.45)$$

To determine the extreme points of $\Lambda(N)$ it suffices to consider the values of

$$F(s) = \sum_{k=1}^{N+1} \frac{\alpha_k}{s-z_k} \qquad (6.46)$$

as the α_k and z_k vary according to (6.45). We mention that this rational form for F in (6.46) was essentially the starting point of the analyses given by Bergman and Milton. Their assumption was valid in the above sense.

A convenient way to carry out the determination of the boundary of $\Lambda(N)$ is to use fractional linear transformations of F(s). If $\mu^{(0)} = a_1$ and $\mu^{(1)} = a_2$ are known, i.e., if the first two terms of the $\frac{1}{s}$ power series for F are known,

$$F(s) = \frac{a_1}{s} + \frac{a_2}{s^2} + \cdots \qquad (6.47)$$

then

$$F_1(s) = \frac{1}{a_1} - \frac{1}{sF(s)} \qquad (6.48)$$

is a function of type (6.42) with its $\frac{1}{s}$ power series known only to first order

$$F_1(s) = \frac{a_2/a_1^2}{s} + \cdots \quad . \tag{6.49}$$

The transformation (6.48) can be iterated to reduce a function known to n^{th} order to a function known to first order. This first order function is then easily extremized. We shall use this procedure in the next two sections to obtain bounds on ε^*. Bergman [e.g., 9] was the first to use a variant of this idea to obtain bounds on ε^* up to second order. G. Baker [25] has previously studied the n^{th} order transformations in the context of Padé approximants to Stieltjes series. G. Milton [11] uses another method to obtain n^{th} order bounds on ε^* which are equivalent to those obtained from variational principles, and are essentially the same as Baker's bounds [37].

We now verify that F_1 in (6.48) has a representation like (6.42). Clearly F_1 maps the upper half plane U into the lower half plane L if and only if the functon sF maps U into L. Now $-F(s)$ is positive definite so that its representing moment sequence $\mu^{(0)}, \mu^{(1)}, \mu^{(2)}, \cdots$ is positive definite. Since

$$sF = \mu^{(0)} + \frac{\mu^{(1)}}{s} + \frac{\mu^{(2)}}{s^2} + \cdots \tag{6.50}$$

and $\mu^{(1)}, \mu^{(2)}, \cdots$ is a positive definite sequence with representing measure $z\mu(dz)$, sF maps U into L. Furthermore, F_1 is analytic off [0,1] since sF does not vanish off [0,1]. In addition, F_1 is analytic at s =

∞ with $F_1(\infty) = 0$. Thus there is a positive Borel measure μ_1 on $[0,1]$ such that

$$F_1(s) = \int_0^1 \frac{\mu_1(dz)}{s - z} . \tag{6.51}$$

Before we obtain the bounds on ε^* we mention two properties of F and its measure μ. For the special case of rational F as in (6.46), the zeroes and poles of F interlace. Let $\xi_1, \xi_2, \cdots, \xi_{N+1}$ be the zeroes of $1 - F$. Consideration of $\frac{1}{m}$ renders them between 0 and 1 in the s-plane. Then

$$1 - \sum_{k=1}^{N+1} \frac{\alpha_k}{s - z_k} = \prod_{k=1}^{N+1} \frac{s - \xi_k}{s - z_k} , \tag{6.52}$$

so that

$$0 \leqslant \alpha_p = - \frac{\prod_{k=1}^{N+1} (z_p - \xi_k)}{\prod_{k \neq p} (z_p - z_k)} , \quad p = 1, 2, \cdots, N+1 . \tag{6.53}$$

This implies that

$$0 \leqslant z_{N+1} \leqslant \xi_{N+1} \leqslant \cdots \leqslant \xi_2 \leqslant z_1 \leqslant \xi_1 \leqslant 1. \tag{6.54}$$

We examine the condition given by Bergman [3] as

$$F(1) \leqslant 1. \tag{6.55}$$

By $s = 1$ we mean $\varepsilon_1 = 0$ with ε_2 fixed off $(-\infty, 0)$. For μ as in (6.44) the meaning of (6.55) is clear. The z_k are not allowed to equal 1, and both the α_k and z_k are constrained by

$$\sum_{k=1}^{N+1} \frac{\alpha_k}{1 - z_k} \leqslant 1. \tag{6.56}$$

By the Krein-Milman theorem any measure in M can be expressed as a weak* limit of convex combinations of one-point masses. Thus for the effective parameter problem we must restrict out attention to measures in M that are weak* limits of discrete measures obeying (6.56). Clearly for such measures μ,

$$\int_0^1 \frac{\mu(dz)}{1 - z} \leqslant 1. \tag{6.57}$$

Using the Dominated Convergence theorem we can now compute F(1). Since

$$g_n(z) = \sum_{i=0}^{n} z^i \leqslant \frac{1}{1 - z} \tag{6.58}$$

and $g_n(z) \to 1/(1-z)$ almost everywhere in $[0,1]$,

$$\lim_{n\to\infty} \int_0^1 \sum_{i=0}^{n} z_i^n \, \mu(dz) = \int_0^1 \frac{\mu(dz)}{1 - z} \quad . \tag{6.59}$$

Thus

$$F(1) = \sum_{n=0}^{\infty} \mu^{(n)}. \tag{6.60}$$

D. Real Bounds

We assume that $s > 1$ is fixed with $0 < \varepsilon_1 < \varepsilon_2$. If only the volume fractions p_1 and p_2 are known then $F = 1 - \frac{\varepsilon^*}{\varepsilon_2}$ is known to first order

$$F(s) = \frac{p_1}{s} + \cdots \tag{6.61}$$

so that $\mu^{(0)} = p_1$. Evaluating (6.42) with a point measure of mass p_1 gives

$$F(s) = \frac{p_1}{s-z}\ , \quad 0 \leq z \leq p_2. \tag{6.62}$$

To minimize (6.73) z is set to 0,

$$F(s) \geq \frac{p_1}{s}\ . \tag{6.63}$$

In terms of ε^*, (6.63) is the upper Wiener bound

$$\varepsilon^* \leq p_1\varepsilon_1 + p_2\varepsilon_2. \tag{6.64}$$

To obtain the lower bound on ε^* we consider the function

$$E(s) = 1 - \frac{\varepsilon_1}{\varepsilon^*}\ . \tag{6.65}$$

Bergman [9] has made use of E(s) and the other dual functions $1 - \frac{\varepsilon_2}{\varepsilon^*}$

and $1 - \frac{\varepsilon^*}{\varepsilon_1}$ associated with F in obtaining real and complex bounds on ε^* to second order. Milton [11] has used a similar idea in the derivation of his n^{th} order real and complex bounds, and has pointed out to the author that all of his bounds can be obtained through analysis of only F and E. Clearly E(s) has an integral representation like that of F(s),

$$E(s) = \int_0^1 \frac{\nu(dz)}{s-z} . \tag{6.66}$$

In addition

$$E(s) = \frac{1-sF(s)}{s(1-F(s))} , \tag{6.67}$$

and in the sense of the previous section,

$$E(1) \leqslant 1. \tag{6.68}$$

To first order,

$$E(s) = \frac{p_2}{s} + \cdots \quad . \tag{6.69}$$

Evaluating (6.66) with a point measure of mass p_2 gives

$$E(s) = \frac{p_2}{s-z} , \; 0 \leqslant z \leqslant p_1. \tag{6.70}$$

Minimizing gives

$$E(s) \geqslant \frac{p_2}{s} . \tag{6.71}$$

Combining (6.71) with (6.64) gives the Wiener bounds,

$$\frac{1}{\frac{p_1}{\varepsilon_1} + \frac{p_2}{\varepsilon_2}} \leqslant \varepsilon^* \leqslant p_1\varepsilon_1 + p_2\varepsilon_2 . \tag{6.72}$$

These bounds are optimal. The upper bound can be attained by a composite of slabs of the two materials ε_1 and ε_2 of volume fractions p_1 and p_2 aligned parallel to the applied field. The lower bound is attained by the slab geometry arranged perpendicular to the field.

If the material is further assumed to be statistically isotropic then the Wiener bounds can be improved. In this case F is known to second order

$$F(s) = \frac{p_1}{s} + \frac{p_1 p_2}{ds^2} + \cdots \quad . \tag{6.73}$$

Applying the transformation (6.48)

$$F_1(s) = \frac{1}{p_1} - \frac{1}{sF(s)} \tag{6.74}$$

gives to first order

$$F_1(s) = \frac{p_2}{p_1 ds} + \cdots \quad . \tag{6.75}$$

Evaluating (6.51) with a point measure of mass $p_2/(p_1 d)$ yields

$$F_1(s) = \frac{p_2/(p_1 d)}{s - z} \; , \; 0 \leqslant z \leqslant \frac{d-1}{d} \; . \qquad (6.76)$$

The minimum of (6.76) is

$$F_1(s) \geqslant \frac{p_2/(p_1 d)}{s} \; . \qquad (6.77)$$

In terms of F(s),

$$F(s) \geqslant \frac{p_1}{s - p_2/d} \; , \qquad (6.78)$$

and in terms of ε^* (6.78) is the upper Hashin-Shtrikman bound,

$$\varepsilon^* \leqslant \varepsilon_2 + \frac{p_1}{\frac{1}{\varepsilon_1 - \varepsilon_2} + \frac{p_2}{d\varepsilon_2}} \; . \qquad (6.79)$$

To obtain the lower bound on ε^*, note that to second order

$$E(s) = \frac{p_2}{s} + \frac{p_1 p_2 (d-1)}{ds^2} + \cdots \; . \qquad (6.80)$$

Now let

$$E_1(s) = \frac{1}{p_2} - \frac{1}{sE(s)} \tag{6.81}$$

so that to first order

$$E_1(s) = \frac{p_1(d-1)}{p_2 ds} + \cdots \quad . \tag{6.82}$$

Since $E_1(s)$ has the representation

$$E_1(s) = \int_0^1 \frac{\nu_1(dz)}{s-z} , \tag{6.83}$$

we let ν_1 be a point measure of mass $p_1(d-1)/(p_2 d)$,

$$E_1(s) = \frac{p_1(d-1)/(p_2 d)}{s - z} , \quad 0 \leq z \leq \frac{1}{d} \quad . \tag{6.84}$$

Minimizing,

$$E_1(s) \geq \frac{p_1(d-1)}{p_2 ds} \tag{6.85}$$

or

$$E(s) \geq \frac{p_2}{s - \frac{p_1(d-1)}{d}} \quad . \tag{6.86}$$

Combining (6.86) for ε^* and (6.79) gives the Hashin-Shtrikman bounds

$$\varepsilon_1 + \frac{p_2}{\frac{1}{\varepsilon_2-\varepsilon_1} + \frac{p_1}{d\varepsilon_1}} \leqslant \varepsilon^* \leqslant \varepsilon_2 + \frac{p_1}{\frac{1}{\varepsilon_1-\varepsilon_2} + \frac{p_2}{d\varepsilon_2}}, \ \varepsilon_1 \leqslant \varepsilon_2. \tag{6.87}$$

Like the Wiener bounds, these bounds are optimal. The upper bound is attained when the composite consists of densely packed spheres of all sizes composed of material 1 coated with material 2 in the appropriate volume fraction. The lower bound is attained by switching the roles of materials 1 and 2.

It is interesting to note that the bound on F induced by the transformation F_1 is equivalent to Hölder's inequality, and similarly for E. We can write (6.78) as

$$F(s) \geqslant \frac{\mu^{(0)}}{s - \mu^{(1)}/\mu^{(0)}} \quad . \tag{6.88}$$

With

$$F(s) = \frac{\mu^{(0)}}{s} + \frac{\mu^{(1)}}{s^2} + \frac{\mu^{(2)}}{s^3} + \frac{\mu^{(3)}}{s^4} + \cdots \quad , \tag{6.89}$$

(6.88) can be rewritten as

$$\frac{\mu^{(0)}}{s} + \frac{\mu^{(1)}}{s^2} + \frac{\mu^{(2)}}{s^3} + \frac{\mu^{(3)}}{s^4} + \cdots \geqslant \frac{\mu^{(0)}}{s} + \frac{\mu^{(1)}}{s^2} + \frac{(\mu^{(1)})^2}{\mu^{(0)}s^3} + \frac{(\mu^{(1)})^3}{(\mu^{(0)})^2 s^4} + \cdots \quad . \tag{6.90}$$

For third order and higher, the bound can be written term by term as

$$(\mu^{(1)})^k \leq (\mu^{(0)})^{k-1} \mu^{(k)} \quad , \ k \geq 2 \qquad (6.91)$$

which is equivalent to Hölder's inequality

$$\int_0^1 z\ \mu(dz) \leq \left(\int_0^1 \mu(dz)\right)^{\frac{k-1}{k}} \left(\int_0^1 z^k\ \mu(dz)\right)^{1/k} . \qquad (6.92)$$

To demonstrate iteration of the transformations F_1 and E_1 we derive third order bounds on ε^*. Assume

$$F(s) = \frac{a_1}{s} + \frac{a_2}{s^2} + \frac{a_3}{s^3} + \cdots \qquad (6.93)$$

and

$$F_1(s) = \frac{1}{a_1} - \frac{1}{s\ F(s)} . \qquad (6.94)$$

To second order,

$$F_1(s) = \frac{a_2}{a_1^2 s} + \left(\frac{a_3}{a_1^2} - \frac{a_2^2}{a_1^3}\right) \frac{1}{s^2} + \cdots \quad . \qquad (6.95)$$

Now let

$$F_2(s) = \frac{a_1^2}{a_2} - \frac{1}{s\,F_1(s)}\ , \tag{6.96}$$

so that to first order

$$F_2(s) = a_1\left(\frac{a_1 a_3}{a_2^2} - 1\right)\frac{1}{s} + \cdots\ . \tag{6.97}$$

Since F_2 has the representation

$$F_2(s) = \int_0^1 \frac{\mu_2(dz)}{s - z}\ , \tag{6.98}$$

we can minimize F_2 by letting μ_2 be a point measure at $z = 0$ of mass $a_1\left(\frac{a_1 a_3}{a_2^2} - 1\right)$,

$$F_2(s) \geq \frac{a_1\left(\frac{a_1 a_3}{a_2^2} - 1\right)}{s}\ . \tag{6.99}$$

In terms of F, (6.99) is

$$F(s) \geq \frac{a_1}{s - \cfrac{s}{\cfrac{a_1}{a_2}s + 1 - \cfrac{a_1 a_3}{a_2^2}}}\ , \tag{6.100}$$

and in terms of ε^*,

$$\varepsilon^* \leqslant \varepsilon_2 + \cfrac{a_1}{\cfrac{1}{\varepsilon_1 - \varepsilon_2} + \cfrac{a_2/a_1}{\varepsilon_2 + \left(\frac{a_2}{a_1} - \frac{a_3}{a_2}\right)(\varepsilon_2 - \varepsilon_1)}} . \tag{6.101}$$

Note that (6.101) with $a_1 = p_1$ and $a_2 = p_1 p_2/d$ is a better bound than (6.78) since $\left(\frac{a_2}{a_1} - \frac{a_3}{a_2}\right) \leqslant 0$, which is just the Schwartz inequality.

The lower bound is obtained from transforming

$$E(s) = \frac{b_1}{s} + \frac{b_2}{s^2} + \frac{b_3}{s^3} + \cdots \tag{6.102}$$

first by

$$E_1(s) = \frac{1}{b_1} - \frac{1}{sE(s)} . \tag{6.103}$$

As in (6.96), let

$$E_2(s) = \frac{b_1^2}{b_2} - \frac{1}{sE_1(s)} , \tag{6.104}$$

with

$$E_2(s) = \int_0^1 \frac{\nu_2(dz)}{s - z} \tag{6.105}$$

and

$$E_2(s) = b_1\left(\frac{b_1 b_3}{b_2^2} - 1\right)\frac{1}{s} + \cdots \quad . \tag{6.106}$$

Minimizing (6.105) gives

$$E_2(s) \geqslant b_1\left(\frac{b_1 b_3}{b_2^2} - 1\right)\frac{1}{s} \quad . \tag{6.107}$$

The lower bound corresponding to (6.101) is

$$\varepsilon^* \geq \cfrac{1}{\cfrac{1}{\varepsilon_1} + \cfrac{b_1}{\cfrac{1}{\cfrac{1}{\varepsilon_2} - \cfrac{1}{\varepsilon_1}} + \cfrac{b_2/b_1}{\cfrac{1}{\varepsilon_1} + \left(\cfrac{b_2}{b_1} - \cfrac{b_3}{b_2}\right)\left(\cfrac{1}{\varepsilon_1} - \cfrac{1}{\varepsilon_2}\right)}}} \quad . \tag{6.108}$$

In [11] Milton points out that these bounds and the higher order bounds obtained from more iterations of F_1 and E_1 are optimal. They are not necessarily attained, though, within the class of statistically isotropic materials, because in general these bounds violate the interchange inequality (6.20).

The higher order bounds may be described as follows. Assume

$$F(s) = \frac{a_1}{s} + \frac{a_2}{s^2} + \cdots + \frac{a_n}{s^n} + \cdots \quad . \tag{6.109}$$

Following the iteration procedure outlined above, the last transformation to be used will be

$$F_{n-1}(s) = \frac{1}{\mu_{n-2}^{(0)}} - \frac{1}{sF_{n-2}(s)} , \tag{6.110}$$

with

$$F_i(s) = \int_0^1 \frac{\mu_i(dz)}{s - z} . \tag{6.111}$$

The bound is obtained by letting μ_{n-1} be a point measure at the origin of mass $\mu_{n-1}^{(0)}$,

$$F_{n-1}(s) \geq \frac{\mu_{n-1}^{(0)}}{s} , \tag{6.112}$$

where the $\mu_i^{(0)}$ can be computed from the a_i as the iteration proceeds. There is a large literature within the theory of Padé approximants which covers the determination of such quantities as $\mu_i^{(0)}$ [25, 26, 27]. In terms of F, (6.112) is a continued fraction

$$F(s) \geq \cfrac{1}{\cfrac{s}{\mu^{(0)}} - \cfrac{s}{\cfrac{s}{\mu_1^{(0)}} - \cfrac{s}{\cfrac{s}{\mu_2^{(0)}} - \cfrac{s}{\vdots \atop \cfrac{s}{\mu_{n-2}^{(0)}} - \mu_{n-1}^{(0)}}}}} . \tag{6.113}$$

This lower bound on F gives an upper bound on ε^*. The lower bound on ε^* arises from applying the same considerations to E(s), known to n^{th} order.

E. Complex Bounds

Now fix $s \in \mathbb{C}$ with $\operatorname{Im} s \neq 0$. We first give bounds assuming no information about the mixture geometry. Since

$$F(s) = \int_0^1 \frac{\mu(dz)}{s - z}, \tag{6.114}$$

the extremal values of F are attained when μ is a point measure of mass ≤ 1 concentrated in $[0,1)$,

$$F(s) = \frac{\alpha}{s-z}, \quad 0 \leq \alpha \leq 1, \quad 0 \leq z < 1. \tag{6.115}$$

Since $F(1) \leq 1$, the allowed region in the F-plane is the image of the triange in (α,z)-space defined by

$$\alpha + z \leq 1, \quad 0 \leq \alpha \leq 1, \quad 0 \leq z < 1 \tag{6.116}$$

under the mapping (6.115). This region is bounded by a circular arc parameterized by

$$C(\alpha) = \frac{\alpha}{s - (1-\alpha)}, \quad 0 \leq \alpha \leq 1, \tag{6.117}$$

and a line segment parameterized by

$$L(\alpha) = \frac{\alpha}{s}, \quad 0 \leq \alpha \leq 1. \tag{6.118}$$

These bounds are optimal. Any point on the line segment can be attained by the slab composite aligned parallel to the field with p_1 =

α. Any point on the arc can be attained by the slab composite aligned perpendicular to the field with $p_1 = \alpha$. The two vertices are attained when the composite consists of only material 1 or of only material 2.

Assuming knowledge of the volume fractions p_1 and $p_2 = 1 - p_1$ we generate a region contained inside that above. The allowed values of F lie inside the circle parameterized by

$$C_1(z) = \frac{p_1}{s-z}, \ -\infty \leqslant z \leqslant \infty. \tag{6.119}$$

On the other hand, the allowed values of E lie inside the circle parameterized by

$$\hat{C}_1(y) = \frac{p_2}{s-y}, \ -\infty \leqslant y \leqslant \infty. \tag{6.120}$$

In the ε^*-plane the intersection of these two regions is bounded by two circular arcs. These arcs correspond to $0 \leqslant z \leqslant p_2$ in (6.119) and $0 \leqslant y \leqslant p_1$ in (6.120). As Bergman [9] and Milton [12] show, these bounds are optimal. Points on the arc of C_1 are attained by composites of spheroidal cores of material 1 in the volume fraction p_1 coated with confocal shells of material 2 in the volume fraction p_2. The spheroids are uniformly aligned with the polar axis parallel to the field and all have the same aspect ratios. In a given sample there are all sizes of spheroids. The arc of C_1 is traced out as the aspect ratio varies. The $\hat{C}_1$ arc is attained by switching the roles of materials 1 and 2 and then allowing the aspect ratio to vary. The vertex $C_1(0)$ is attained when the spheroids have degenerated to cylindrical "cigars" parallel to the field with $F = p_1/s$ (slab parallel) and $\hat{C}_1(0)$ is attained when the spheroids degenerate to "infinite" pancakes perpendicular to the field with $E = p_2/s$ (slab perpendicular). Note that these vertices lie on the arcs from the previous zeroth order bounds. This optimal spheroidal geometry is a generalization of the Hashin-Shtrikman coated sphere geometry.

By further assuming statistical isotropy, F is known to second order as in (6.73). Then F_1 in (6.74) is known to first order. Since F_1 has the representation (6.51) its allowed values lie inside the circle parameterized by

$$C_2(z) = \frac{p_2/(p_1 d)}{s - z}, \ -\infty \leqslant z \leqslant \infty \quad . \tag{6.121}$$

Alternatively the allowed values of E_1 in (6.83) lie inside the circle parameterized by

$$\hat{C}_2(y) = \frac{p_1(d-1)/(p_2 d)}{s - y}, \ -\infty \leqslant y \leqslant \infty. \tag{6.122}$$

Since F is fractional linear in F_1 and E is fractional linear in E_1, the circles C_2 and $\hat{C}_2$ are transformed to circles in the F- and E-planes, parameterized by

$$F_s(z) = \frac{p_1(s - z)}{s(s-z-p_2/d)}, \ -\infty \leqslant z \leqslant \infty, \tag{6.123}$$

$$E_s(y) = \frac{p_2(s - y)}{s(s-y-p_1(d-1)/d)} \quad , -\infty \leqslant y \leqslant \infty. \tag{6.124}$$

In the ε^*-plane the intersection of these two circular regions is bounded by two circular arcs. These arcs correspond to $0 \leqslant z \leqslant (d-1)/d$ in (6.123) and $0 \leqslant y \leqslant \frac{1}{d}$ in (6.124). The vertices of the region, $F(z=0) = p_1/(s - p_2/d)$ and $E(y=0) = p_2/(s - p_1(d-1)/d)$ are attained by the Hashin-Shtrikman geometries (spheres of material 1 and volume fraction p_1 coated with material 2 and vice versa) and lie on the arcs of the first order bounds.

Except for the vertices, the above bounds are not optimal because in general they violate the interchange inequality (6.20). In two dimensions where the inequality becomes an equality, Milton [16] has improved the above bounds. In [10] Bergman gives a treatment of Milton's bounds and extends them to higher dimensions. For two dimensions Bergman writes the Keller interchange equality as

$$A(s) + A(t) = 0 \quad , t = 1-s \tag{6.125}$$

or

$$\frac{A(s)}{s - \frac{1}{2}} = \frac{A(t)}{t - \frac{1}{2}} \quad , \tag{6.126}$$

where

$$A(s) = \frac{s - p_2/d}{p_1} - \frac{1}{F(s)} . \qquad (6.127)$$

It then follows that $A(s)/(s - \frac{1}{2})$ is an even function of $s - \frac{1}{2}$, which leads to the definition of the new positive definite function

$$D(q) = \frac{A(s)}{s - \frac{1}{2}} , \; q = (s - \frac{1}{2})^2 . \qquad (6.128)$$

Extremization of D subject to $F(1) \leq 1$ shows that the allowed values of F lie either inside or outside the circle parameterized by

$$B(z) = \frac{p_1(s - \frac{1}{2})}{(s - \frac{1}{2})(s - \frac{1}{2}p_2) - p_1 z} , \; -\infty \leq z \leq \infty \quad . \qquad (6.129)$$

If $F = \infty$ is allowed then the admissible region is outside the circle and conversely. A similar analysis is applied to E(s) and the resulting circle is

$$\hat{B}(y) = \frac{p_2(s - \frac{1}{2})}{(s - \frac{1}{2})(s - \frac{1}{2}p_1) - p_2 y} , \quad -\infty \leq y \leq \infty \quad . \qquad (6.130)$$

The region obtained in the intersection is bounded by the two circular arcs $0 \leq z \leq p_2/4p_1$ in (6.129) and $0 \leq y \leq p_1/4p_2$ in (6.130). The vertices are the same as before but now the arcs as well are optimal. The arc of B(z) in (6.129) is attained by doubly-coated spheres: a core of ε_2, coated by a spherical shell of ε_1, coated again by a shell of ε_2. The arc of $\hat{B}(y)$ in (6.130) is attained by interchanging materials 1 and 2 in the doubly-coated sphere geometry.

We now describe the n^{th} order complex bounds (neglecting the interchange inequality). Assuming as in the real case that $a_1, \cdots, a_n$ are known, then $F_{n-1}(s)$ is the last transformation to be used in the iteration procedure. Since

$$F_{n-1}(s) = \int_0^1 \frac{\mu_{n-1}(dz)}{s - z} , \qquad (6.131)$$

the allowed values of F_{n-1} lie inside the circle parameterized by

$$C_n(z) = \frac{\mu_{n-1}^{(0)}}{s - z} , \quad -\infty \leq z \leq \infty . \qquad (6.132)$$

Now F is fractional linear in F_{n-1} so that this circle is transformed into a circle in the F-plane,

$$F_z(s) = \cfrac{1}{\cfrac{s}{\mu^{(0)}} - \cfrac{s}{\cfrac{s}{\mu_1^{(0)}} - \cfrac{s}{\cfrac{\vdots}{\cfrac{s}{\mu_{n-2}^{(0)}} - \cfrac{s\mu_{n-1}^{(0)}}{s - z}}}}} , \quad -\infty \leq z \leq \infty . \qquad (6.133)$$

Analysis of E_{n-1} gives a similar circle in the E-plane. The intersection of the two induced circular regions in the ε^*-plane is bounded by two circular arcs. The arc coming from (6.133) is traced out as z varies between 0 and a, where a is determined by the condition that $F(1) \leq 1$, just as in the first and second order bounds; similarly for E. The resulting bounds form a sequence of nested lens-shaped regions, where the vertices of the n^{th} order bound lie on the arcs of the bound of order n-1. Again these bounds are not optimal for isotropic materials because of violation of the interchange inequality. Baker [25, 26] derives a similar set of bounds, differing only in that we bound the dual function E(s) in addition to the original function F(s), so that our bounds on F(s) are tighter than his. As $n \to \infty$, the bounds converge to a point in the complex plane. Physically, this means that if one knows all the correlation functions of the material then the effective parameter is completely characterized.

7. The Polydisc Representation Formula

A. Derivation of the Formula

In section 4 we showed that $m(h_1,h_2) : \tilde{U}^2 \to \{Im(m) > 0\}$. As counterparts of m in $\tilde{U}^2$ we consider analytic functions in the conformally equivalent polydisc $D^2 = \{|\zeta_1| < 1\} \times \{|\zeta_2| < 1\}$ with positive real part there. We will derive the analogue of (6.13) for such functions.

Let $f(\zeta_1,\zeta_2)$ be holomorphic with nonnegative real part in D^2. We first give a polydisc Schwartz formula which expresses f restricted to $D_R^2 = \{|\zeta_1| < R\} \times \{|\zeta_2| < R\}$, $R < 1$, in terms of an integral of its real part over $T_R^2 = \{|w_1| = R\} \times \{|w_2| = R\}$. Cauchy's Formula for $(\zeta_1,\zeta_2) \in D_R^2$ is

$$f(\zeta_1,\zeta_2) = \left(\frac{1}{2\pi i}\right)^2 \iint_{T_R^2} \frac{f(w_1,w_2)}{(w_1-\zeta_1)(w_2-\zeta_2)}\, dw_1 dw_2 \,. \qquad (7.1)$$

Let $\zeta_j^* = (R^2/r_j)e^{i\theta_j}$ be the reflection of $\zeta_j = r_j e^{i\theta_j}$ in the circle $\{|w_j| = R\}$, $j = 1,2$. From the one-variable Cauchy Formula one can see that if ζ_1 or ζ_2 or both are replaced by their reflections in the integral in (7.1), then the integral vanishes. Therefore, $f(\zeta_1,\zeta_2)$ may be written as

$$f(\zeta_1,\zeta_2) = \left(\frac{1}{2\pi i}\right)^2 \iint_{T_R^2} f(w_1,w_2)\left(\frac{1}{w_1-\zeta_1} \pm \frac{1}{w_1-\zeta_1^*}\right)\left(\frac{1}{w_2-\zeta_2} \pm \frac{1}{w_2-\zeta_2^*}\right) dw_1 dw_2 \,, \qquad (7.2)$$

for any combination of +'s and −'s. With $dw_j = iRe^{it_j}dt_j$, we have

$$\left(\frac{1}{w_j-\zeta_j} - \frac{1}{w_j-\zeta_j^*}\right) dw_j = \frac{i(R^2-r_j^2)}{R^2+r_j^2-2r_jR\cos(\theta_j-t_j)} dt_j \tag{7.3}$$

$$\left(\frac{1}{w_j-\zeta_j} + \frac{1}{w_j-\zeta_j^*}\right) dw_j = i\left(1 + \frac{i2r_jR\sin(\theta_j-t_j)}{R^2+r_j^2-2r_jR\cos(\theta_j-t_j)}\right) dt_j. \tag{7.4}$$

Then $f(\zeta_1,\zeta_2)$ has the following equivalent forms

$$f(\zeta_1,\zeta_2) = \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi} f(t_1,t_2)(1+iQ_1)P_2 dt_1 dt_2 \tag{7.5}$$

$$f(\zeta_1,\zeta_2) = \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi} f(t_1,t_2)(1+iQ_2)P_1 dt_1 dt_2 \tag{7.6}$$

$$f(\zeta_1,\zeta_2) = \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi} f(t_1,t_2)(1+iQ_1)(1+iQ_2) dt_1 dt_2 \tag{7.7}$$

$$f(\zeta_1,\zeta_2) = \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi} f(t_1,t_2)P_1P_2 dt_1 dt_2 \tag{7.8}$$

where

$$P_j = \mathrm{Re}[H_j],\ Q_j = \mathrm{Im}[H_j],\ H_j = \frac{w_j+\zeta_j}{w_j-\zeta_j},\ w_j = Re^{it_j}\ . \tag{7.9}$$

With $f = u + iv$, (7.8) gives

$$u(\zeta_1,\zeta_2) = \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi} u(t_1,t_2)P_1P_2dt_1dt_2. \qquad (7.10)$$

Adding (7.5), (7.6) and (7.7) yields

$$3v(\zeta_1,\zeta_2) = \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi} \Big[u(t_1,t_2)(Q_1P_2+Q_2P_1+Q_1+Q_2) + v(t_1,t_2)(P_1+P_2+1-Q_1Q_2)\Big]dt_1dt_2 . \qquad (7.11)$$

Using

$$H_1H_2 = P_1P_2 - Q_1Q_2 + i(P_1Q_2 + P_2Q_1) \qquad (7.12)$$

allows us to write

$$3f = \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi}\Big[u(2P_1P_2 + i(Q_1+Q_2) + H_1H_2) + iv(1+P_1+P_2) + \bar{f}Q_1Q_2\Big]dt_1dt_2 . \qquad (7.13)$$

From (7.7)

$$\left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi} \bar{f}Q_1Q_2dt_1dt_2 = \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi}\Big(\bar{f} - i(Q_1+Q_2)\Big)dt_1dt_2 - \bar{f} , \qquad (7.14)$$

which gives

$$3f = \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi}\Big[u(H_1H_2 + 2P_1P_2 + 1) + v(i(P_1+P_2) - Q_1 - Q_2)\Big]dt_1dt_2 - \bar{f} . \qquad (7.15)$$

In view of (7.10) this becomes

$$2f = \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi} \int_0^{2\pi} \left[u(H_1H_2+1) + v(i(P_1+P_2) - Q_1 - Q_2) \right] dt_1dt_2 \quad . \qquad (7.16)$$

Recalling the single variable Schwartz formula for a function $f(\zeta)$ analytic in the unit disc

$$f(\zeta) = iv(0) + \frac{1}{2\pi} \int_0^{2\pi} \frac{Re^{it} + \zeta}{Re^{it} - \zeta} \; u(Re^{it})dt, \; \zeta = re^{i\theta}, \; r < R < 1 \qquad (7.17)$$

allows (7.16) to be written as

$$2f = \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi} \int_0^{2\pi} u(H_1H_2 - 1)dt_1dt_2 + f(\zeta_1,0) + f(0,\zeta_2) \; , \qquad (7.18)$$

or equivalently,

$$f(\zeta_1,\zeta_2) = iv(0,0) + \frac{1}{2} \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi} \int_0^{2\pi} (H_1H_2 + H_1 + H_2 - 1) \; u(Re^{it_1},Re^{it_2})dt_1dt_2 \; . \qquad (7.19)$$

The representation in (7.19) can be verified by expanding f in a power series

$$f(\zeta_1, \zeta_2) = \sum_{n,m=0}^{\infty} A_{nm} \zeta_1^n \zeta_2^m$$
$$= A_{00} + \sum_{n=1}^{\infty} A_{no} \zeta_1^n + \sum_{m=1}^{\infty} A_{om} \zeta_2^m + \sum_{n,m=1}^{\infty} A_{nm} \zeta_1^n \zeta_2^m \; , \qquad (7.20)$$

which may be written as

$$f(\zeta_1,\zeta_2) = f(0,0) + \left(f(\zeta_1,0) - f(0,0) \right) + \left(f(0,\zeta_2) - f(0,0) \right)$$
$$+ \left(f(\zeta_1, \zeta_2) - f(\zeta_1,0) - f(0, \zeta_2) + f(0,0) \right) . \qquad (7.21)$$

Observing the fact that for n, m ≥ 1,

$$2A_{nm}\zeta_1^n\zeta_2^m = \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi} H_1H_2 \operatorname{Re}[A_{nm} w_1^n w_2^m]\, dt_1 dt_2 , \tag{7.22}$$

and applying the single variable Schwartz formula (7.17) gives (7.19).

We wish to extend (7.19) to the entire polydisc D^2. Define σ_R, an increasing function of t_1 and t_2 separately, by

$$\sigma_R(t_1,t_2) = \left(\frac{1}{2\pi}\right)^2 \int_0^{t_1}\int_0^{t_1} u(Re^{it_1'},Re^{it_2'})\, dt_1'\, dt_2'. \tag{7.23}$$

Since $\sigma_R(2\pi,2\pi) = u(0,0)$ for every $R < 1$, Helly's theorem allows us to pass to the limit as $R \to 1$ and define

$$\sigma(t_1,t_2) = \lim_{R\to 1} \sigma_R(t_1,t_2) \tag{7.24}$$

at all points of continuity of σ. We now have a formula for $f(\zeta_1,\zeta_2)$ valid in D^2,

$$f(\zeta_1,\zeta_2) = iv(0,0) + \frac{1}{2}\iint_{T^2}(H_1H_2 + H_1 + H_2 - 1)\mu(dt_1,dt_2) , \tag{7.25}$$

where μ is the positive Borel measure on T^2 induced by σ.

One should note that not all positive measures on T^2 arise from the boundary values of the positive real parts of holomorphic functions in D^2 [28]. Indeed, for every $R < 1$, $u(Re^{it_1}, Re^{it_2})$ has non-zero Fourier coefficients only in $Z_+^2 \cup Z_-^2$, where $Z_+ = \{0,1,2,\cdots\}$ and $Z_- = -Z_+$. This follows from observing that

$$u = \frac{1}{2}(f + \bar{f}) \tag{7.26}$$

and on T^2, f has the form

$$f(Re^{it_1}, Re^{it_2}) = \sum_{n,m=0}^{\infty} A_{nm} e^{i(nt_1+mt_2)}. \tag{7.27}$$

Since $(\frac{1}{2\pi})^2 u(Re^{it_1}, Re^{it_2})\, dt_1\, dt_2$ converges weak* to $\mu(dt_1, dt_2)$ as $R \to 1$, μ has non-zero Fourier coefficients only in $Z_+^2 \cup Z_-^2$.

We have now proved necessity in the following

Theorem: For $f(\zeta_1, \zeta_2)$ to be holomorphic with nonnegative real part in D^2 it is necessary and sufficient that f may be represented as

$$f(\zeta_1,\zeta_2) = iv(0,0) + \frac{1}{2}\iint_{T^2} \left(\frac{e^{it_1}+\zeta_1}{e^{it_1}-\zeta_1}\,\frac{e^{it_2}+\zeta_2}{e^{it_2}-\zeta_2} + \frac{e^{it_1}+\zeta_1}{e^{it_1}-\zeta_1} + \frac{e^{it_2}+\zeta_2}{e^{it_2}-\zeta_2} - 1\right)\mu(dt_1,dt_2) \tag{7.28}$$

where μ is a positive Borel measure on T^2 satisfying

$$\iint_{T^2} e^{i(nt_1 + mt_2)}\, \mu(dt_1, dt_2) = 0 \text{ unless } (n,m) \in Z_+^2 \cup Z_-^2. \tag{7.29}$$

Sufficiency is proved by first noting that the integral in (7.28) gives rise to a holomorphic function in D^2. This can be seen by expanding (7.28) in powers of ζ_1 and ζ_2, where $|\zeta_1| < 1$ and $|\zeta_2| < 1$. Then the power series generated by (7.28) converges uniformly on compact subsets of D^2. That the real part of (7.28) is positive follows from writing (7.10) as

$$\mathrm{Re}[f(\zeta_1,\zeta_2)] = u(\zeta_1,\zeta_2) = \iint_{T^2} P_1 P_2 \,\mu(dt_1,dt_2) \tag{7.30}$$

where P_1 and P_2 are positive.

Representations of $f(\zeta_1,\zeta_2)$ equivalent to (7.28) have been given by Korányi and Pukánzky in [29] and by Vladimirov and Drozhzhinov in [30]. Korányi and Pukánszky prove that f may be represented by

$$f(\zeta_1,\zeta_2) = iv(0,0) + \iint_{T^2} (2S(\zeta_1,\zeta_2,w_1,w_2) - 1)\,\mu(dt_1,dt_2) \tag{7.31}$$

where μ satisfies (7.29) and S is the Szëgo kernel

$$S = \frac{1}{(1 - \frac{\zeta_1}{w_1})(1 - \frac{\zeta_2}{w_2})} \quad . \tag{7.32}$$

A little algebra shows that

$$2S - 1 = \frac{1}{2}(H_1H_2 + H_1 + H_2 - 1) \ , \tag{7.33}$$

as it must.

B. Reproduction of the Boundary Values

We now verify that the kernel $\frac{1}{2}(H_1H_2 + H_1 + H_2 - 1)$ reproduces the "boundary values" of the function it represents. That is, we show that as (ζ_1,ζ_2) are sent radially to $(\tilde{\zeta}_1, \tilde{\zeta}_2) \in T^2_R$, the right hand side of (7.19) converges to $f(\tilde{\zeta}_1, \tilde{\zeta}_2)$. To do this we use the single variable results [31] that

$$\lim_{r_j \to R} \frac{1}{2\pi} \int_0^{2\pi} P_j \; u \; dt_j = u(\tilde{\zeta}_j) \tag{7.34}$$

$$\lim_{r_j \to R} \frac{1}{2\pi} \int_0^{2\pi} Q_j \; u \; dt_j = v(\tilde{\zeta}_j) - v(0) \tag{7.35}$$

First letting $r_1 \to R$ in (7.19) yields

$$\begin{aligned} \lim_{r_1 \to R} f(\zeta_1,\zeta_2) &= iv(0,0) + \tfrac{1}{2}\left(u(\tilde{\zeta}_1,0) + i(v(\tilde{\zeta}_1,0) - v(0,0))\right) \\ &+ \tfrac{1}{2}\left(\tfrac{1}{2\pi}\right) \int_0^{2\pi} [P_2 u(\tilde{\zeta}_1,t_2) - Q_2(v(\tilde{\zeta}_1,t_2) - v(0,t_2))] \\ &+ i[Q_2\, u(\tilde{\zeta}_1,t_2) + P_2(v(\tilde{\zeta}_1,t_2) - v(0,t_2))]\, dt_2. \end{aligned} \tag{7.36}$$

Now letting $r_2 \to R$ as well yields

$$\begin{aligned} \lim_{r_1,r_2 \to R} f(\zeta_1,\zeta_2) &= \tfrac{1}{2}\left(f(\tilde{\zeta}_1,0) + f(0,\tilde{\zeta}_2)\right) - \tfrac{1}{2} u(0,0) \\ &+ \tfrac{1}{2}\left(u(\tilde{\zeta}_1,\tilde{\zeta}_2) + u(\tilde{\zeta}_1,\tilde{\zeta}_2) - u(\tilde{\zeta}_1,0) + u(0,0) - u(0,\tilde{\zeta}_2)\right) \\ &+ \tfrac{i}{2}\left(v(\tilde{\zeta}_1,\tilde{\zeta}_2) - v(\tilde{\zeta}_1,0) + v(\tilde{\zeta}_1,\tilde{\zeta}_2) - v(0,\tilde{\zeta}_2)\right). \end{aligned} \tag{7.37}$$

Thus (7.19) reproduces the boundary values of f on T_R^2 ,

$$\lim_{r_1,r_2 \to R} f(\zeta_1,\zeta_2) = f(\tilde{\zeta}_1,\tilde{\zeta}_2). \tag{7.38}$$

We conclude that if in some region of T^2, μ has a density that is say, continuous, then taking radial limits of the real part of (7.28) reproduces the values of the density in the region.

C. Boundary Behavior where the Measure Vanishes

From (4.10) we have that when h_1 and h_2 are real, $m(h_1,h_2)$ is necessarily analytic only when both h_1 and h_2 are positive. It then follows that the measure μ in (7.28) can have no mass on the subset E of T^2 which corresponds to $\mathbb{R}_+^2$ in (h_1,h_2)-space. In order to use (7.28) for $(\zeta_1,\zeta_2) \in E$ we should verify that as (ζ_1,ζ_2) is sent radially to E, the real part of (7.28) vanishes identically on E, and that (7.28) gives rise to a purely imaginary analytic function on E. Note that in Section B above we have already shown the first of these two statements, but we will reprove it here.

An extension of f into $(D^*)^2 = \{|\zeta_1| > 1\} \times \{|\zeta_2| > 1\}$ is given by

$$f(\zeta_1^*,\zeta_2^*) = \overline{f(\zeta_1,\zeta_2)} \quad . \tag{7.39}$$

Let A_1 denote f in D^2 and A_2 denote f in $(D^*)^2$. Now $\left(\frac{1}{2\pi}\right)^2$ $u(Re^{it_1}, Re^{it_2})$ $dt_1 dt_2$ converges weak* to $\mu(dt_1,dt_2)$ as $R \to 1$. Thus as radial limits are taken, A_1 and A_2 converge in the sense of distributions to the same purely imaginary limit. The edge of the wedge theorem [32] then gives the existence of a function A holomorphic in a neighborhood $\mathcal{N} \subset \mathbb{C}^2$ of E containing $D^2 \cup (D^*)^2$ such that $A|_{D^2} = A_1$ and $A|_{(D^*)^2} = A_2$. Then $A|_E$ is a purely imaginary analytic function on E.

It is interesting to note that if μ is allowed to have point masses off E, then the above statements are not in general true.

However, this "non-localization" which may occur in D^n, $n \geqslant 2$, is prevented by the Fourier condition (7.29), as Rudin [33] points out.

We now find an expression for the purely imaginary $A|_E$ in the case that μ has a continuous density $m(t_1,t_2)$. Under this assumption we write

$$f(\zeta_1,\zeta_2) = iv(0,0) + \frac{1}{2}\left(\frac{1}{2\pi}\right)^2 \iint_{T^2} (H_1H_2 + H_1 + H_2 - 1)m(t_1,t_2)dt_1dt_2. \qquad (7.40)$$

We assume for convenience that $E = (\pi, 2\pi) \times (\pi, 2\pi)$. The H_1 and H_2 integrals in (7.40) can be written as

$$\begin{aligned} f(\zeta_1,\zeta_2) = iv(0,0) &+ \frac{1}{2}\left(\frac{1}{2\pi}\right) \int_0^{2\pi} H_1 m_1(t_1)dt_1 + \frac{1}{2}\left(\frac{1}{2\pi}\right) \int_0^{2\pi} H_2 m_2(t_2)dt_2 \\ &+ \frac{1}{2}\left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi} (H_1H_2 - 1)\, m(t_1,t_2)dt_1dt_2 , \end{aligned} \qquad (7.41)$$

where

$$m_1(t_1) = \frac{1}{2\pi}\int_0^{2\pi} m(t_1,t_2)dt_2, \quad m_2(t_2) = \frac{1}{2\pi}\int_0^{2\pi} m(t_1,t_2)dt_1. \qquad (7.42)$$

By (7.38) with $R = 1$ the imaginary part of (7.28) converges to $A|_E$ in the radial limit. Then it suffices to analyze

$$\begin{aligned} v(\zeta_1,\zeta_2) = iv(0,0) &+ \frac{i}{2}\left(\frac{1}{2\pi}\right) \int_0^{2\pi} Q_1 m_1(t_1)dt_1 + \frac{i}{2}\left(\frac{1}{2\pi}\right) \int_0^{2\pi} Q_2 m_2(t_2)dt_2 \\ &+ \frac{i}{2}\left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi} (P_1Q_2 + P_2Q_1)\, m(t_1,t_2)dt_1dt_2. \end{aligned} \qquad (7.43)$$

Since the first two integrals in (7.43) are single variable functions we may immediately set r_1 and r_2 to 1 in their kernels [31]. We focus on

$$I(r_1e^{i\theta_1},r_2e^{i\theta_2}) = \left(\frac{1}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi} P_1Q_2\, m(t_1,t_2)dt_1dt_2\ , \qquad (7.44)$$

which can be written as

$$I(r_1e^{i\theta_1},r_2e^{i\theta_2}) = \left(\frac{1}{2\pi}\right)^2 \left[\int_0^{2\pi}\int_0^{\pi} P_1Q_2mdt_1dt_2 + \int_0^{\pi}\int_0^{2\pi} P_1Q_2m\, dt_1dt_2 - \int_0^{\pi}\int_0^{\pi} P_1Q_2mdt_1dt_2\right]. \qquad (7.45)$$

Since P_1 behaves as $r_1 \to 1$ as a delta function concentrated at $t_1 = \theta_1$, where $\pi < \theta_1 < 2\pi$, the last two integrals in (7.45) may be set to zero in the radial limit. Now applying (7.34) for a continuous weight with $R = 1$ gives

$$\lim_{r_1,r_2\to 1} I(r_1e^{i\theta_1},r_2e^{i\theta_2}) = I(e^{i\theta_1},e^{i\theta_2}) = \frac{1}{2\pi}\int_0^{2\pi} Q_2\, m(\theta_1,t_2)dt_2\ . \qquad (7.46)$$

Thus we write

$$\lim_{r_1,r_2\to 1} f(r_1e^{i\theta_1},r_2e^{i\theta_2}) = f(e^{i\theta_1},e^{i\theta_2}) \qquad (7.47)$$

with

$$f(e^{i\theta_1},e^{i\theta_2}) = iv(0,0) + \frac{i}{2}\left(\frac{1}{2\pi}\right)\left[\int_0^{2\pi} Q_1\big(m_1(t_1) + m(t_1,\theta_2)\big)dt_1 + \int_0^{2\pi} Q_2\big(m_2(t_2) + m(\theta_1,t_2)\big)dt_2\right]. \qquad (7.48)$$

Since $H_1 = iQ_1$ and $H_2 = iQ_2$ for $(\zeta_1,\zeta_2) \in T^2$,

$$f(e^{i\theta_1},e^{i\theta_2}) = iv(0,0) + \frac{1}{2}\left(\frac{1}{2\pi}\right)\left[\int_0^{2\pi} \frac{e^{it_1}+e^{i\theta_1}}{e^{it_1}-e^{i\theta_1}}\left(m_1(t_1) + m(t_1,\theta_2)\right) dt_1 + \right.$$

$$\left.\int_0^{2\pi} \frac{e^{it_2}+e^{i\theta_2}}{e^{it_2}-e^{i\theta_2}}\left(m_2(t_2) + m(\theta_1,t_2)\right) dt_2\right]. \qquad (7.49)$$

Now m satisfies (7.29) and vanishes on $E = (\pi,2\pi) \times (\pi,2\pi)$. From the edge of the wedge argument f in (7.49) is analytic in $e^{i\theta_1}$ and $e^{i\theta_2}$ when $(\theta_1,\theta_2) \in E$. Consequently

$$B(e^{i\theta_1}, e^{i\theta_2}) = \int_0^{2\pi} \frac{e^{it_1} + e^{i\theta_1}}{e^{it_1} - e^{i\theta_1}} m(t_1,\theta_2)\, dt_1 \;, \; \pi < \theta_1,\theta_2 < 2\pi \qquad (7.50)$$

is analytic in $e^{i\theta_2}$ as well as $e^{i\theta_1}$ when $(\theta_1,\theta_2) \in E$, and similarly for 1 and 2 reversed. Because m vanishes on E, $m(t_1,\theta_2)$ vanishes when $\pi < t_1 < 2\pi$. In addition

$$C(e^{i\theta_1}) = \int_0^{2\pi} \frac{e^{it_1} + e^{i\theta_1}}{e^{it_1} - e^{i\theta_1}} m_1(t_1)dt_1 \;, \quad \pi < \theta_1 < 2\pi \qquad (7.51)$$

is analytic and purely imaginary in $e^{i\theta_1}$, $\pi < \theta_1 < 2\pi$. When $\pi < t_1 < 2\pi$, $m_1(t_1)$ is the real part of $C(e^{i\theta_1})$. Thus $m_1(t_1)$ vanishes in $\pi < t_1 < 2\pi$. The same holds for $m_2(t_2)$.

In the general case where μ is a positive measure vanishing on E and satisfying (7.29), we have on E,

$$f(e^{i\theta_1},e^{i\theta_2}) = iv(0,0) + \frac{1}{2}\Big[\int_0^{\pi} H_1\big(\mu_1(dt_1) + \mu_{\theta_2}(dt_1)\big) + \int_0^{\pi} H_2\big(\mu_2(dt_2) + \mu_{\theta_1}(dt_2)\big)\Big]. \qquad (7.52)$$

The measures in (7.52) are obtained from the following radial weak* limits of $u = \mathrm{Re}[f]$,

$$\mu_1(dt_1) = \lim_{R\to 1}\Big(\int_0^{2\pi} u(Re^{it_1},Re^{it_2})dt_2\Big)\,dt_1 \qquad (7.53)$$

$$\mu_{\theta_2}(dt_1) = \lim_{R\to 1} u(Re^{it_1},Re^{i\theta_2})dt_1\ , \qquad (7.54)$$

and similarly for μ_2 and μ_{θ_2}. The mass restrictions on μ_1 and μ_{θ_2} induced by the above considerations for μ with continuous density have been included in (7.52). Again, we have that

$$B(e^{i\theta_1},e^{i\theta_2}) = \int_0^{\pi} \frac{e^{it_1} + e^{i\theta_1}}{e^{it_1} - e^{i\theta_1}}\mu_{\theta_2}(dt_1)\ , \pi < \theta_1,\theta_2 < 2\pi \qquad (7.55)$$

is analytic in $e^{i\theta_2}$ as well as $e^{i\theta_1}$, and that

$$C(e^{i\theta_1}) = \int_0^{\pi} \frac{e^{it_1} + e^{i\theta_1}}{e^{it_1} - e^{i\theta_1}}\mu_1(dt_1)\ ,\quad \pi < \theta_1 < 2\pi \qquad (7.56)$$

is analytic in $e^{i\theta_1}$. Similarly for μ_{θ_1} and μ_2.

Let us develop (7.55) into a power series representation. With $w_1 = e^{it_1}$, $\zeta_1 = e^{i\theta_1}$ and $\zeta_2 = e^{i\theta_2}$, we have

$$B(\zeta_1,\zeta_2) = \mu^{(o)}_{\theta_2} + 2[\mu^{(1)}_{\theta_2}\zeta_1 + \mu^{(2)}_{\theta_2}\zeta_1^2 + \cdots] , \tag{7.57}$$

where

$$\mu^{(n)}_{\theta_2} = \int_0^{\pi} (\frac{1}{w_1})^n \mu_{\theta_2}(dt_1). \tag{7.58}$$

Now each $\mu^{(n)}_{\theta_2}$ is an analytic function of $\zeta_2 = e^{i\theta_2}$, so that it has a power series

$$\mu^{(n)}_{\theta_2} = \sum_{j=0}^{\infty} a_j^{(n)} (\theta_2 - \theta^*)^j , \qquad \theta^* \in (\pi, 2\pi). \tag{7.59}$$

The $a_j^{(n)}$ are the n^{th} moments of "j^{th} derivative" measures

$$a_j^{(n)} = \int_0^{\pi} (\frac{1}{w_1})^n \mu_{\theta_2,j}(dt_1), \tag{7.60}$$

where the limit in the derivatve

$$\mu_{\theta_2,j} = \frac{\partial^j \mu_{\theta_2}}{\partial \theta_2^j}\Big|_{\theta_2 = \theta^*} \tag{7.61}$$

holds in the weak* sense. These "j^{th} derivative" measures have the following equivalent definition,

$$\mu_{\theta_2,j}(dt_1) = \lim_{R\to 1} [\frac{\partial^j u}{\partial \theta_2^j} (Re^{it_1}, Re^{i\theta_2})dt_1]\Big|_{\theta_2 = \theta^*} , \tag{7.62}$$

where the limit is taken in the weak* sense.

8. Bounds for Three-Component Media

A. The Perturbation Expansion and its Analytic Continuation

For $|s_1| > 1$ and $|s_2| > 1$ we can expand (5.9) with $i = k$ about a homogeneous medium ($s_1 = s_2 = \infty$),

$$F(s_1,s_2) = \int_\Omega P(d\omega)\Big[\Big(\frac{\chi_1}{s_1} + \frac{\chi_2}{s_2} - \frac{\chi_1\Gamma\chi_1}{s_1^2} - \frac{\chi_2\Gamma\chi_2}{s_2^2} - \frac{(\chi_1\Gamma\chi_2 + \chi_2\Gamma\chi_1)}{s_1 s_2} + \cdots\Big) e_k\Big] \cdot e_k . \tag{8.1}$$

If only the volume fractions p_1, p_2 and $p_3 = 1 - p_1 - p_2$ are known then F is known to first order

$$F(s_1,s_2) = \frac{p_1}{s_1} + \frac{p_2}{s_2} + \cdots \quad . \tag{8.2}$$

As in the two-component case, the second order terms can be calculated by assuming statistical isotropy of the medium. Let

$$c_{ij} = \int_\Omega P(d\omega)\, \chi_i\, \Gamma_{kk}\, \chi_j \quad , \; i,j = 1,2. \tag{8.3}$$

Again we can write

$$c_{ij} = \int_{\mathbb{R}^d} G_{kk}(y)\, R_{ij}(y) dy \; , \tag{8.4}$$

where $G_{kk}(y)$ is the kernel of the singular integral operator A_{kk} of (6.16) and

$$R_{ij}(y) = \int_\Omega P(d\omega)\, \chi_i(x+y,\omega)\big(\chi_j(x,\omega) - p_j\big) . \tag{8.5}$$

Under the statistical isotropy assumption,

$$c_{ij} = \frac{-R_{ij}(0)}{d}, \tag{8.6}$$

where

$$R_{ij}(0) = \begin{cases} -p_1 p_2 & i \neq j \\ \\ p_i - p_i^2 & i = j. \end{cases} \tag{8.7}$$

Thus to second order,

$$F(s_1,s_2) = \frac{p_1}{s_1} + \frac{p_2}{s_2} + \frac{p_1-p_1^2}{ds_1^2} + \frac{p_2-p_2^2}{ds_2^2} - \frac{2p_1p_2}{ds_1s_2} + \cdots \quad . \tag{8.8}$$

Consider $f(\zeta_1,\zeta_2)$ on D^2, the counterpart to $F(s_1,s_2)$ on $U^2 = \{\mathrm{Im}\, s_1 > 0\} \times \{\mathrm{Im}\, s_2 > 0\}$. The perturbation expansion (8.1) about $s_1 = s_2 = \infty$ corresponds to a Taylor expansion of $f(\zeta_1,\zeta_2)$ about $\zeta_1 = \zeta_2 = 1$, which is in the region of T^2 where the measure vanishes. As could be anticipated from the power series development of f in (7.52) through (7.57), the way in which (7.28) provides the analytic continuation of (8.1) is not as simple as in the two-component case. Mapping (7.52) with E the complement of $\big((\pi, 3\pi/2) \times [0,2\pi)\big) \cup \big([0,2\pi) \times (\pi, 3\pi/2)\big)$ to U^2 gives

$$K(s_1,s_2) = -\gamma + \frac{1}{2}\int_0^1 \frac{1 + z_1 s_1}{z_1 - s_1}\left(\mu_1(dz_1) + \mu_{s_2}(dz_1)\right)$$

$$+ \frac{1}{2}\int_0^1 \frac{1 + z_2 s_2}{z_2 - s_2}\left(\mu_2(dz_2) + \mu_{s_1}(dz_2)\right) \ , \tag{8.9}$$

where $K(s_1,s_2) = -F(s_1,s_2) = if(\zeta_1,\zeta_2)$ and $\gamma = v(0,0)$. Rename $\mu_1(dz_2) = \mu_2(dz_2) + \mu_{s_1}(dz_2)$ and $\mu_2(dz_1) = \mu_1(dz_1) + \mu_{s_2}(dz_1)$ so that

$$K(s_1,s_2) = -\gamma + \frac{1}{2}\int_0^1 \frac{1 + z_1 s_1}{z_1 - s_1}\mu_2(dz_1) + \frac{1}{2}\int_0^1 \frac{1 + z_2 s_2}{z_2 - s_2}\mu_1(dz_2) \ . \tag{8.10}$$

Recall that $F(\infty,\infty) = -K(\infty,\infty) = 0$. Then

$$-\gamma = \frac{1}{2}\int_0^1 z_1 \, \mu_{2\infty}\,(dz_1) + \frac{1}{2}\int_0^1 z_2 \, \mu_{1\infty}\,(dz_2) \ , \tag{8.11}$$

where

$$\mu_{1\infty} = \mu_1\big|_{s_1 = \infty}$$

$$\mu_{2\infty} = \mu_2\big|_{s_2 = \infty} \ . \tag{8.12}$$

Since

$$\frac{1 + z_1 s_1}{z_1 - s_1} = -\left(z_1 + \frac{(1 + z_1^2)}{s_1} + \frac{z_1(1 + z_1^2)}{s_1^2} + \cdots\right) \tag{8.13}$$

we may write

$$K(s_1,s_2) = \frac{1}{2}\int_0^1 z_1\big(\mu_{2\,\infty}(dz_1) - \mu_2(dz_1)\big) + \frac{1}{2}\int_0^1 z_2\big(\mu_{1\,\infty}(dz_2) - \mu_1(dz_2)\big)$$

$$- \frac{1}{2}\int_0^1\Big(\frac{1}{s_1} + \frac{z_1}{s_1^2} + \frac{z_1^2}{s_1^3} + \cdots\Big)\,\nu_2(dz_1) - \frac{1}{2}\int_0^1\Big(\frac{1}{s_2} + \frac{z_2}{s_2^2} + \frac{z_2^2}{s_2^3} + \cdots\Big)\nu_1(dz_2), \qquad (8.14)$$

where $\nu_1 = (1 + z_2^2)\mu_1$ and $\nu_2 = (1 + z_1^2)\mu_2$. Now expand μ_1 and ν_1 in powers of $1/s_2$,

$$\mu_1 = \mu_{1\,\infty} + \sum_{j=1}^{\infty} \frac{\mu_{1,j}}{s_1^j} \qquad (8.15)$$

$$\nu_1 = \nu_{1\,\infty} + \sum_{j=1}^{\infty} \frac{\nu_{1,j}}{s_2^j}$$

and similarly for μ_2 and ν_2, where the $\mu_{1,j}$ and $\nu_{1,j}$ are the j^{th} derivative measures analogous to (7.61). In terms of $F = -\,K$, (8.14) becomes

$$F(s_1,s_2) = \frac{1}{2}\Big[\sum_{j=1}^{\infty}\Big(\frac{\mu_{2,j}^{(1)} + \nu_{2\,\infty}^{(j-1)}}{s_2^j} + \frac{\mu_{1,j}^{(1)} + \nu_{1\,\infty}^{(j-1)}}{s_1^j}\Big) \qquad (8.16)$$

$$+ \sum_{j,k=1}^{\infty} \frac{\nu_{2,k}^{(j-1)} + \nu_{1,j}^{(k-1)}}{s_1^j s_2^k}\Big].$$

To second order,

$$F(s_1,s_2) = \frac{1}{2}\Big[\frac{\mu^{(1)}_{2,1} + \nu^{(o)}_{2\infty}}{s_2} + \frac{\mu^{(1)}_{1,1} + \mu^{(o)}_{1\infty}}{s_1}$$

$$+ \frac{\mu^{(1)}_{2,2} + \nu^{(1)}_{2\infty}}{s_2^2} + \frac{\mu^{(1)}_{1,2} + \nu^{(1)}_{1\infty}}{s_1^2} + \frac{\nu^{(o)}_{2,1} + \nu^{(o)}_{1,1}}{s_1 s_2} + \cdots\Big] \quad . \tag{8.17}$$

B. The Representation of Certain Extremals

Let $K : U^2 \to \{\mathrm{Im}\ K > 0\}$ vanish at and be analytic in a neighborhood of (∞, ∞). Furthermore let K be such that its counterpart on D^2 arises from a sum of product measures of the form

$$\mu(dt_1,dt_2) = \mu_1(dt_1) \times \frac{dt_2}{2\pi} + \frac{dt_1}{2\pi} \times \mu_2(dt_2) \ , \tag{8.18}$$

where μ_1 and μ_2 are positive Borel measures on $(\pi, 3\pi/2)$, not to be confused with those from the previous section. The mass restriction on μ_1 and μ_2 gives the correct domain of analyticity for $F = -K$ on U^2.

The reason why we are interested in functions arising from (8.18) is as follows. For two-component media the bounds were obtained by examining the images of extreme points of the positive measures with fixed mass under the mapping (6.42). Let

$$M_a = \{\text{positive Borel measures } \mu \text{ on } T^2 \text{ satisfying the Fourier condition (7.29) and } \iint_{T^2} \mu(dt_1,dt_2) = a > 0\}. \tag{8.19}$$

The simplest extreme points of M_a have the form

$$\mu_1^* = a\,\delta_{t_1^*} \times \frac{dt_2}{2\pi}\,,\quad \mu_2^* = a\,\delta_{t_2^*} \times \frac{dt_1}{2\pi}\,, \tag{8.20}$$

where $0 \leq t_1^*, t_2^* < 2\pi$. The image of μ_1^* under (7.28) as t_1^* varies between 0 and 2π is a circle lying in $\{\mathrm{Re}\ f > 0\}$. The image of μ_2^* under (7.28) as t_2^* varies is a circle in $\{\mathrm{Re}\ f > 0\}$ which either contains or is contained by the μ_1^* circle. If $|\zeta_1| < |\zeta_2|$ then the μ_2^* circle contains the μ_1^* circle. Now the full set of extreme points of M_a has not been completely characterized [33,34,35]. However, we conjecture that the image of M_a under (7.28) lies inside the larger of the two circles from μ_1^* and μ_2^*. Using this ansatz in the next two sections we will rederive classical real bounds for three-component materials and obtain new complex bounds. In the appendix we will discuss this conjecture for a discrete approximation of M_a. In particular, we will show that for our discrete model of M_1, the only extreme points are discrete versions of the measures in (8.20).

We now find a formula for $K(s_1,s_2)$ arising from (8.18). Evaluating (7.28) with μ as in (8.18) and $\gamma = v(0,0)$ gives

$$f(\zeta_1,\zeta_2) = i\gamma + \tfrac{1}{2}\Big[\Big(\int_{\pi}^{3\pi/2} H_1\mu_1(dt_1)\Big)\Big(\frac{1}{2\pi}\int_0^{2\pi} H_2 dt_2\Big) + \int_{\pi}^{3\pi/2} H_1\mu_1(dt_1) + \frac{1}{2\pi}\int_0^{2\pi} H_2 dt_2 - 1\Big]$$

$$+ \tfrac{1}{2}\Big[\Big(\int_{\pi}^{3\pi/2} H_2\mu_2(dt_2)\Big)\Big(\frac{1}{2\pi}\int_0^{2\pi} H_1 dt_1\Big) + \int_{\pi}^{3\pi/2} H_2\mu_2(dt_2) + \frac{1}{2\pi}\int_0^{2\pi} H_1 dt_1 - 1\Big]. \quad (8.21)$$

The function

$$b = u + iv = \frac{1}{2\pi}\int_0^{2\pi} \frac{w_1 + \zeta_1}{w_1 - \zeta_1} dt_1 \quad (8.22)$$

is analytic on $|\zeta_1| < 1$ with $u = 1$ and $v = 0$ on $|\zeta_1| = 1$ and $u = 1$ and $v = 0$ at $\zeta_1 = 0$. The maximum modulus principle yields $b \equiv 1$. Thus

$$f(\zeta_1,\zeta_2) = i\gamma + \int_{\pi}^{3\pi/2} \frac{w_1 + \zeta_1}{w_1 - \zeta_1}\mu_1(dt_1) + \int_{\pi}^{3\pi/2} \frac{w_2 + \zeta_2}{w_2 - \zeta_2}\mu_2(dt_2). \quad (8.23)$$

Letting $K(s_1,s_2) = i\, f(\zeta_1,\zeta_2)$ with $\zeta_j = (s_j - i)/(s_j + i)$ and $w_j = (z_j - i)/(z_j + i)$ gives

$$K(s_1,s_2) = -\gamma + \int_0^1 \frac{1 + z_1 s_1}{z_1 - s_1}\mu_1(dz_1) + \int_0^1 \frac{1 + z_2 s_2}{z_2 - s_2}\mu_2(dz_2), \quad (8.24)$$

where $\mu_1(dz_1)$ and $\mu_2(dz_2)$ are positive Borel measures on $[0,1]$. Further imposing that $K(\infty,\infty) = 0$ forces

$$-\gamma = \int_0^1 z_1\mu_1(dz_1) + \int_0^1 z_2\mu_2(dz_2), \quad (8.25)$$

which allows (8.24) to be written as

$$K(s_1,s_2) = \int_0^1 \frac{(1+z_1^2)}{z_1-s_1}\mu_1(dz_1) + \int_0^1 \frac{(1+z_2^2)}{z_2-s_2}\mu_2(dz_2). \tag{8.26}$$

Absorbing $(1 + z_1^2)$ and $(1 + z_2^2)$ into μ_1 and μ_2 without renaming gives

$$K(s_1,s_2) = \int_0^1 \frac{\mu_1(dz_1)}{z_1 - s_1} + \int_0^1 \frac{\mu_2(dz_2)}{z_2 - s_2} \quad . \tag{8.27}$$

We will let K represent various functions associated with F to derive bounds.

C. Real Bounds

Since $F : U^2 \to \{\text{Im } F < 0\}$ its counterpart in D^2 has a representation like (7.28). To find extremal values of F we look in the class of measures (8.18) so that with K = – F in (8.27),

$$F(s_1,s_2) = \int_0^1 \frac{\mu_1(dz_1)}{s_1-z_1} + \int_0^1 \frac{\mu_2(dz_2)}{s_2-z_2} \quad . \tag{8.28}$$

If only the volume fractions p_1, p_2 and p_3 are known then to first order,

$$F(s_1,s_2) = \frac{p_1}{s_1} + \frac{p_2}{s_2} + \cdots \quad . \tag{8.29}$$

Equating (8.29) to the $1/s_1$ and $1/s_2$ expansion of (8.28) forces

$$\mu_1^{(o)} = p_1 \quad , \mu_2^{(o)} = p_2 \; . \tag{8.30}$$

Letting $\mu_1 = p_1\delta_{a_1}$ and $\mu_2 = p_2\delta_{a_2}$ as in (8.20) gives

$$F(s_1,s_2) = \frac{p_1}{s_1-a_1} + \frac{p_2}{s_2-a_2}, \quad 0 \leq a_1,a_2 < 1. \tag{8.31}$$

In (8.31) we have set a_1 and a_2 strictly less than 1 because analogous to (6.55), $F(s_1,s_2)$ must obey the condition $F(1,1) \leq 1$. To minimize $F(s_1,s_2)$ for fixed $s_1,s_2 > 1$ we set $a_1 = a_2 = 0$,

$$F(s_1,s_2) \geq \frac{p_1}{s_1} + \frac{p_2}{s_2}, \tag{8.32}$$

which is equivalent to the upper Wiener bound

$$\varepsilon^* \leq p_1\varepsilon_1 + p_2\varepsilon_2 + p_3\varepsilon_3 \tag{8.33}$$

with $\varepsilon_1 \leq \varepsilon_2 \leq \varepsilon_3$.

To obtain the lower bound on ε^* we consider

$$H(t_1,t_2) = 1 - \varepsilon_3/\varepsilon^* = F(s_1,s_2)/\big(F(s_1,s_2) - 1\big), \tag{8.34}$$

where $t_1 = 1 - s_1$ and $t_2 = 1 - s_2$. We could also use $1 - \varepsilon_2/\varepsilon^*$. Since $H(t_1,t_2)$: $\{\text{Im } t_1 > 0\} \times \{\text{Im } t_2 > 0\} \to \{\text{Im } H < 0\}$ its counterpart in D^2 has a representation like (7.28). In addition, $H(t_1,t_2)$ has the same region of analyticity as $F(s_1,s_2)$ so that to get extremal values of H we restrict our attention to

$$H(t_1,t_2) = \int_0^1 \frac{\mu_1(dz_1)}{t_1-z_1} + \int_0^1 \frac{\mu_2(dz_2)}{t_2-z_2}\ , \tag{8.35}$$

where μ_1 and μ_2 are again positive Borel measures on [0,1]. To first order H has the expansion

$$H(t_1,t_2) = \frac{p_1}{t_1} + \frac{p_2}{t_2} + \cdots\ . \tag{8.36}$$

To minimize (8.35) we set $\mu_1 = p_1\delta_{a_1}$ and $\mu_2 = p_2\delta_{a_2}$ with $a_1 = a_2 = 0$ so that

$$H(t_1,t_2) \geqslant \frac{p_1}{t_1} + \frac{p_2}{t_2}\ . \tag{8.37}$$

Collecting our two bounds (8.33) and (8.37) gives the classical Wiener bounds for three-component materials

$$\frac{1}{\frac{p_1}{\varepsilon_1} + \frac{p_2}{\varepsilon_2} + \frac{p_3}{\varepsilon_3}} \leqslant \varepsilon^* \leqslant p_1\varepsilon_1 + p_2\varepsilon_2 + p_3\varepsilon_3. \tag{8.38}$$

These bounds are optimal and are attained by the slab geometries of ε_1, ε_2 and ε_3.

If the material is further assumed to be statistically isotropic then F is known to second order as in (8.8),

$$F(s_1,s_2) = \frac{p_1}{s_1} + \frac{p_2}{s_2} + \frac{p_1-p_1^2}{ds_1^2} + \frac{p_2-p_2^2}{ds_2^2} - \frac{2p_1p_2}{ds_1s_2} + \cdots \quad . \tag{8.39}$$

Note that there arises in (8.39) a non-zero second order cross term $-2p_1p_2/ds_1s_2$ so that (8.27) is not directly applicable. However, consider the function

$$G(s_1,s_2) = \frac{F(s_1,s_2)}{1 - \frac{1}{d} F(s_1,s_2)} \; . \tag{8.40}$$

Now $G(s_1,s_2) : U^2 \to \{\mathrm{Im}\, G < 0\}$ and has the same domain of analyticity as $F(s_1,s_2)$, so that it has a representation like (7.28) in D^2. To second order $G(s_1,s_2)$ has the expansion

$$G(s_1,s_2) = \frac{p_1}{s_1} + \frac{p_2}{s_2} + \frac{p_1}{ds_1^2} + \frac{p_2}{ds_2^2} + \frac{0}{s_1s_2} + \cdots \quad . \tag{8.41}$$

The important point to note is that there is no second order cross-term in (8.41) so that now the extremal values of G can be obtained by letting $K = - G$ in (8.27),

$$G(s_1,s_2) = \int_0^1 \frac{\mu_1(dz_1)}{s_1 - z_1} + \int_0^1 \frac{\mu_2(dz_2)}{s_2 - z_2} \; . \tag{8.42}$$

Letting $\mu_1 = p_1\delta_{a_1}$ and $\mu_2 = p_2\delta_{a_2}$ gives

$$G(s_1,s_2) = \frac{p_1}{s_1-a_1} + \frac{p_2}{s_2-a_2}\ , \quad 0 \leqslant a_1,a_2 < 1 \tag{8.43}$$

where a_1 and a_2 have been set strictly less than 1 because $F(1,1) \leqslant 1$ implies that $G(1,1) \leqslant d/(d-1)$. Comparison of (8.43) with (8.41) forces $a_1 = a_2 = 1/d$, so that for fixed $s_1,s_2 > 1$,

$$G(s_1,s_2) \geqslant \frac{p_1}{s_1 - \frac{1}{d}} + \frac{p_2}{s_2 - \frac{1}{d}}\ . \tag{8.44}$$

In terms of $F(s_1,s_2)$,

$$F(s_1,s_2) \geqslant \frac{1}{\dfrac{1}{\dfrac{p_1}{s_1-1/d} + \dfrac{p_2}{s_2-1/d}} + \dfrac{1}{d}}\ , \tag{8.45}$$

which is equivalent to

$$\varepsilon^* \leq \varepsilon_3 + \frac{1}{\dfrac{1}{\dfrac{p_1}{\dfrac{1}{\varepsilon_1-\varepsilon_3} + \dfrac{1}{d\varepsilon_3}} + \dfrac{p_2}{\dfrac{1}{\varepsilon_2-\varepsilon_3} + \dfrac{1}{d\varepsilon_3}}} - \dfrac{1}{d\varepsilon_3}}\ , \tag{8.46}$$

the Hashin-Shtrikman upper bound with $\varepsilon_1 \leqslant \varepsilon_2 \leqslant \varepsilon_3$.

To obtain the lower bound we consider

$$\tilde{F}(q_2,q_3) = 1 - \varepsilon^*/\varepsilon_1\ , \tag{8.47}$$

where

$$q_2 = \frac{1}{1 - \frac{\varepsilon_2}{\varepsilon_1}}, \quad q_3 = \frac{1}{1 - \frac{\varepsilon_3}{\varepsilon_1}} \quad . \tag{8.48}$$

The function $\tilde{F}(q_2, q_3)$ is the same type as F and has a second order expansion

$$\tilde{F}(q_2,q_3) = \frac{p_2}{q_2} + \frac{p_3}{q_3} + \frac{p_2 - p_2^2}{dq_2^2} + \frac{p_3 - p_3^2}{dq_3^2} - \frac{2p_1p_2}{dq_2q_3} + \cdots \quad . \tag{8.49}$$

Analogous to the treatment for the upper bound we consider

$$\tilde{G}(q_2,q_3) = \frac{\tilde{F}(q_2,q_3)}{1 - \frac{1}{d}\tilde{F}(q_2,q_3)} , \tag{8.50}$$

which takes $\{\text{Im } q_2 > 0\} \times \{\text{Im } q_3 > 0\}$ into $\{\text{Im } \tilde{G} < 0\}$ so that it has a representation like (7.28) in D^2. To second order,

$$\tilde{G}(q_2,q_3) = \frac{p_2}{q_2} + \frac{p_3}{q_3} + \frac{p_2}{dq_2^2} + \frac{p_3}{dq_3^2} + \frac{0}{q_2q_3} + \cdots \quad . \tag{8.51}$$

To obtain extremal values of $\tilde{G}$ we apply (8.27) with $K = -\tilde{G}$,

$$\tilde{G}(q_2,q_3) = \int_0^1 \frac{\mu_1(dz_1)}{q_2 - z_1} + \int_0^1 \frac{\mu_2(dz_2)}{q_3 - z_2} \, . \tag{8.52}$$

Letting $\mu_1 = p_2 \delta_{a_1}$ and $\mu_2 = p_3 \delta_{a_3}$ gives

$$\tilde{G}(q_2, q_3) = \frac{p_2}{q_2 - a_1} + \frac{p_3}{q_3 - a_2} . \qquad (8.53)$$

With $\varepsilon_1 \leqslant \varepsilon_2 \leqslant \varepsilon_3$ we have q_2, $q_3 \leqslant 0$. Comparison of (8.53) with (8.51) forces $a_1 = a_2 = 1/d$ so that for $q_2, q_3 \leqslant 0$,

$$\tilde{G}(q_2, q_3) \leqslant \frac{p_2}{q_2 - \frac{1}{d}} + \frac{p_3}{q_3 - \frac{1}{d}} . \qquad (8.54)$$

In terms of ε^* our two bounds (8.54) and (8.46) become

$$\varepsilon_1 + \frac{1}{\frac{1}{A_1} - \frac{1}{d\varepsilon_1}} \leqslant \varepsilon^* \leqslant \varepsilon_3 + \frac{1}{\frac{1}{A_3} - \frac{1}{d\varepsilon_3}} \qquad (8.55)$$

$$A_j = \sum_{\ell=1}^{3} \frac{p_\ell}{\frac{1}{\varepsilon_\ell - \varepsilon_j} + \frac{1}{d\varepsilon_j}} .$$

These inequalities are the classical Hashin-Shtrikman bounds for three-component materials.

The bounds in (8.55) are attainable for certain volume fractions [36]. The geometry that attains them is a generalization of the coated-spheres discussed for two-component media. The upper bound is attained by a mixture of all different sized spheres of ε_1 and ε_2 each coated with ε_3 in the correct volume fraction. The lower bound is attained by the same mixture with ε_1 and ε_3 reversed. Now let ε_L^* denote the lower bound and ε_U^* denote the upper bound. Then Milton [36] shows that the condition that must be satisfied for the above geometry to attain ε_U^* is that $\varepsilon_2 \leq \varepsilon_U^*$. Furthermore, $\varepsilon_L^* \leq \varepsilon_2$ must hold in order that the lower bound be attained. This suggests that for certain volume fractions the Hashin-Shtrikman bounds for three or more components can be improved.

E. Complex Bounds

We first derive complex bounds on ε^* assuming no information about the material aside from s_1 and s_2, which both lie in the upper half plane (or lower half plane). Since F has a representation like that in (7.28) in D^2, we obtain its extremal values by letting μ_1 and μ_2 in (8.27) be point masses so that

$$F(s_1,s_2) = \frac{\alpha_1}{s_1-z_1} + \frac{\alpha_2}{s_2-z_2} , \tag{8.56}$$

where

$$\alpha_1 + \alpha_2 \leq 1,\ \alpha_1,\alpha_2 \geq 0\ ,\ 0 \leq z_1,z_2 < 1\ ,F(1,1) \leq 1. \tag{8.57}$$

Part of the boundary of the allowed region in the F-plane can be obtained by setting either $\alpha_1 = 0$ or $\alpha_2 = 0$. If $\alpha_2 = 0$, then one of the two following arcs lies on the boundary of the allowed region. The first is the line segment joining the origin and $1/s_1$ parameterized by

$$L_1(\alpha_1) = \frac{\alpha_1}{s_1}, \quad 0 \leq \alpha_1 \leq 1. \tag{8.58}$$

The second is the circular arc joining 0 and $\frac{1}{s_1}$ obtained by setting $F(1,1) = 1$ (with $\alpha_2 = 0$), and is parameterized by

$$C_1(\alpha_1) = \frac{\alpha_1}{s_1 - (1-\alpha_1)}, \quad 0 \leq \alpha_1 \leq 1. \tag{8.59}$$

Repeating this procedure for $\alpha_1 = 0$ gives two arcs joining 0 and $\frac{1}{s_2}$ parameterized by

$$L_2(\alpha_2) = \frac{\alpha_2}{s_2}, \quad 0 \leq \alpha_2 \leq 1 \tag{8.60}$$

$$C_2(\alpha_2) = \frac{\alpha_2}{s_2 - (1-\alpha_2)}, \quad 0 \leq \alpha_2 \leq 1. \tag{8.61}$$

One can apply the above argument to $\tilde{F}(q_2,q_3) = 1 - \varepsilon^*/\varepsilon_1$ to obtain a line segment and a circular arc, each of which join $1/s_1$ and $1/s_2$. The other segment and arc produced by $\tilde{F}(q_2,q_3)$ will be the same as one of those pairs from $F(s_1,s_2)$.

In the F-plane the allowed region may be described as follows. Let T_L be the triangular region lying inside the three line segments above with vertices 0, $1/s_1$ and $1/s_2$. Let T_C be the curved triangular region lying inside the three circular arcs above with vertices 0, $1/s_1$, and $1/s_2$. Then the allowed region is the union of T_L and T_C.

As Milton [pers. comm.] points out, these bounds have a simple interpretation in the ε^*-plane and are easily shown to be optimal. Now let T_L be the triangular region bounded by the line segments

$$\begin{aligned} L_{12}(\alpha) &= \alpha\varepsilon_1 + (1-\alpha)\varepsilon_2 \\ L_{23}(\alpha) &= \alpha\varepsilon_2 + (1-\alpha)\varepsilon_3 \qquad (8.62) \\ L_{13}(\alpha) &= \alpha\varepsilon_1 + (1-\alpha)\varepsilon_3\,, \quad 0 \leq \alpha \leq 1\,. \end{aligned}$$

Let T_C be the curved triangular region bounded by the circular arcs

$$\begin{aligned} C_{12}(\alpha) &= 1/\left(\frac{\alpha}{\varepsilon_1} + \frac{(1-\alpha)}{\varepsilon_2}\right) \\ C_{23}(\alpha) &= 1/\left(\frac{\alpha}{\varepsilon_2} + \frac{(1-\alpha)}{\varepsilon_3}\right) \qquad (8.63) \\ C_{13}(\alpha) &= 1/\left(\frac{\alpha}{\varepsilon_1} + \frac{(1-\alpha)}{\varepsilon_3}\right)\,, \quad 0 \leq \alpha \leq 1. \end{aligned}$$

Each circular arc $C_{ij}(\alpha)$ passes through ε_i, ε_j and the origin. The allowed region is again the union of T_L and T_C. Each segment and arc is attainable. The line segment L_{ij} is attained by a slab geometry parallel to the field composed only of materials i and j in the volume fractions α and $1-\alpha$. The circular arc C_{ij} is attained by the same slab geometry but arranged perpendicular to the field.

If the volume fractions p_1, p_2 and p_3 are known as well as s_1 and s_2, then $F(s_1, s_2)$ is known to first order

$$F(s_1,s_2) = \frac{p_1}{s_1} + \frac{p_2}{s_2} + \cdots \quad . \tag{8.64}$$

We obtain extremal values of $F(s_1,s_2)$ by letting $\mu_1 = p_1\delta_{z_1}$ and $\mu_2 = p_2\delta_{z_2}$ in (8.27) with $F = -K$,

$$F(s_1,s_2) = \frac{p_1}{s_1-z_1} + \frac{p_2}{s_2-z_2} \, . \tag{8.65}$$

Now the allowed values of $F = 1 - \varepsilon^*/\varepsilon_3$ lie inside the region R_3 generated by (8.65) as both z_1 and z_2 vary in $[-\infty, \infty]$. The region R_3 can be constructed as follows. First note that $p_1/(s_1-z_1)$ and $p_2/(s_2-z_2)$ with $-\infty \leqslant z_1, z_2 \leqslant \infty$ are both circles in the lower half plane that contain the origin and are thus tangential to the real axis. To construct R_3 one adds to each point $p_1/(s_1-z_1)$ the circle $p_2/(s_2-z_2)$, $-\infty \leqslant z_2 \leqslant \infty$. The outside boundary of R_3 is a circle characterized by

$$\arg\left(\frac{\partial F}{\partial z_1}\right) = \arg\left(\frac{\partial F}{\partial z_2}\right) \quad , \tag{8.66}$$

with F as in (8.65), where "arg" denotes argument. From (8.66),

$$\arg\left(\frac{p_1}{(s_1-z_1)^2}\right) = \arg\left(\frac{p_2}{(s_2-z_2)^2}\right) , \tag{8.67}$$

or

$$\arg(s_1 - z_1) = \arg(s_2 - z_2) \ . \tag{8.68}$$

With $s_1 = a_1 + ib_1$ and $s_2 = a_2 + ib_2$ we have

$$\tan^{-1}\left(\frac{b_1}{a_1 - z_1}\right) = \tan^{-1}\left(\frac{b_2}{a_2 - z_2}\right) \ , \tag{8.69}$$

or

$$z_2 = \frac{b_2}{b_1} z_1 + \left(a_2 - \frac{b_2 a_1}{b_1}\right) \ . \tag{8.70}$$

Thus the outside boundary $C_3(z_1)$ of R_3 is the image of the line (8.70) in (z_1, z_2)-space under (8.65) and can be paramaterized by

$$C_3(z_1) = \frac{p_1 + p_2 \frac{b_1}{b_2}}{s_1 - z_1} \ , \ -\infty \leqslant z_1 \leqslant \infty. \tag{8.71}$$

Note that $C_3(z_1)$ is a positive multiple of the circle $p_1/(s_1 - z_1)$, $-\infty \leqslant z_1 \leqslant \infty$.

The above argument yielding a circular region can be applied to each of the following six functions

$$\begin{aligned} &1 - \varepsilon^*/\varepsilon_3 \ , \quad 1 - \varepsilon_3/\varepsilon^* \ , \\ &1 - \varepsilon^*/\varepsilon_2 \ , \quad 1 - \varepsilon_2/\varepsilon^* \ , \\ &1 - \varepsilon^*/\varepsilon_1 \ , \quad 1 - \varepsilon_1/\varepsilon^* \ . \end{aligned} \tag{8.72}$$

We focus on $H(t_1,t_2) = 1 - \varepsilon_3/\varepsilon^*$, $t_1 = 1 - s_1$, $t_2 = 1 - s_2$. It is the same type of function as $F(s_1,s_2)$ so that its extremal values are attained when

$$H(t_1,t_2) = \frac{p_1}{t_1-z_1} + \frac{p_2}{t_2-z_2}, \tag{8.73}$$

where we have assumed the first order expansion (8.36). Now note that from the geometrical construction of $C_1(z_1)$, in the F-plane it passes through the imaginary axis at 0 and $-i(p_1/b_1 + p_2/b_2)$. Likewise, the outer boundary of the region generated by (8.73) is a circle in the upper half plane which passes through the imaginary axis at 0 and $i(p_1/b_1 + p_2/b_2)$. Since

$$\frac{1}{F} = 1 - \frac{1}{H}, \tag{8.74}$$

in the F-plane these circles are identical, up to parameterization. Thus it suffices to consider only three functions $1 - \varepsilon^*/\varepsilon_3$, $1 - \varepsilon^*/\varepsilon_2$, and $1 - \varepsilon^*/\varepsilon_1$.

From the following considerations we will eliminate one of these functions. The variables of these functions are

$$1 - \frac{\varepsilon^*}{\varepsilon_3}(s_1,s_2) \quad , \; s_1 = \frac{1}{1 - \frac{\varepsilon_1}{\varepsilon_3}} \; , \; s_2 = \frac{1}{1 - \frac{\varepsilon_2}{\varepsilon_3}}$$

$$1 - \frac{\varepsilon^*}{\varepsilon_2}(r_1, r_3) \quad , \; r_1 = \frac{1}{1 - \frac{\varepsilon_1}{\varepsilon_2}} \; , \; r_3 = \frac{1}{1 - \frac{\varepsilon_3}{\varepsilon_2}} \tag{8.75}$$

$$1 - \frac{\varepsilon^*}{\varepsilon_1}(q_2, q_3) \quad , \; q_2 = \frac{1}{1 - \frac{\varepsilon_2}{\varepsilon_1}} \; , \; q_3 = \frac{1}{1 - \frac{\varepsilon_3}{\varepsilon_1}} \; .$$

For convenience assume that ε_1, ε_2 and ε_3 are in the upper half plane with $\arg \varepsilon_3 < \arg \varepsilon_2 < \arg \varepsilon_1$. Then both s_1 and s_2 are in U and both q_2 and q_3 are in L, while $r_1 \in$ U but $r_2 \in$ L. Because the functions we consider are defined on U^2 or L^2, we disregard the function $1 - \varepsilon^*/\varepsilon_2$ to obtain the crudest first order bounds. Better bounds can be given by considering $1 - \varepsilon^*/\varepsilon_2$ on the domain of analyticity given in section 4, which is more general than U^2 or L^2.

In the ε^*-plane the regions R_3 and R_1 induced by $1 - \varepsilon^*/\varepsilon_3$ and $1 - \varepsilon^*/\varepsilon_1$ become circular regions R_3^* and R_1^*. In the $(1 - \varepsilon^*/\varepsilon_1)$-plane the circular boundary of R_1 can be parameterized by

$$C_1(z_1) = \frac{p_2 + p_3 \frac{\text{Im}\, q_2}{\text{Im}\, q_3}}{q_2 - z_1} \; , \; -\infty \leq z_1 \leq \infty \; . \tag{8.76}$$

The complex first order bound in the ε^*-plane is the intersection of R_1^*, R_3^* and the zeroth order bound $(T_L \cup T_C)$ given above.

We discuss the optimality of the above bounds. Let us focus on $1 - \varepsilon^*/\varepsilon_3$. Recall that for an actual material, z_1 and z_2 in (8.65) are restricted by

$$F(1,1) \leqslant 1, \; 0 \leqslant z_1, \; z_2 < 1. \tag{8.77}$$

These conditions define a corner of the unit square in (z_1,z_2)-space. This region A is bounded by the line segments $(0,0) \to (p_3/(1-p_2),0)$ and $(0,0) \to (0,p_3/(1-p_1))$ and the hyperbolic arc defined by $p_1/(1-z_1) + p_2/(1-z_2) = 1$, $0 \leqslant z_1,z_2 < 1$. If the line (8.70) passes through $(z_1,z_2) = (0,0)$ then at least one point on the circle $C_3(z_1)$ is attainable, namely by the simplest slab geometry parallel to the field with $F = p_1/s_1 + p_2/s_2$ or $\varepsilon^* = p_1\varepsilon_1 + p_2\varepsilon_2 + p_3\varepsilon_3$. In general this arithmetic mean lies inside the two circular arcs $C_1(z_1)$ and $C_3(z_1)$. If the line (8.70) passes through the interior of the region A in (z_1,z_2)-space then the following geometry attains that section of $C_3(z_1)$ [G. Milton, pers. comm.]. Expression (8.65) can be written as

$$\varepsilon^* = \varepsilon_3 + \frac{p_1\varepsilon_3(\varepsilon_1 - \varepsilon_3)}{\varepsilon_3 + z_1(\varepsilon_1 - \varepsilon_3)} + \frac{p_2\varepsilon_3(\varepsilon_2 - \varepsilon_3)}{\varepsilon_3 + z_2(\varepsilon_2 - \varepsilon_3)} \, , \tag{8.78}$$

which is equivalent to

$$\varepsilon^* = (1 - \frac{p_1}{1-z_1} + \frac{p_2}{1-z_2})\,\varepsilon_3 + (\frac{p_1}{1-z_1})\,\frac{1}{\frac{1-z_1}{\varepsilon_1} + \frac{z_1}{\varepsilon_3}}$$

$$+ (\frac{p_2}{1-z_2})\,\frac{1}{\frac{1-z_2}{\varepsilon_2} + \frac{z_2}{\varepsilon_3}} \, . \tag{8.79}$$

This last expression is clearly the effective dielectric constant of a composite consisting of slabs of three materials parallel to the field in the volume fractions $(1- p_1/(1-z_1) - p_2/(1-z_2))$, $(p_1/(1-z_1))$, and $(p_2/(1-z_2))$. The first material is just ε_3. The second is a slab composite perpendicular to the field composed of ε_1 in the volume fraction $1 - z_1$ and ε_3 in the volume fraction z_1. The third is a slab composite perpendicular to the field composed of ε_2 in the volume fraction $1 - z_2$ and ε_3 in the volume fraction z_2. The attained arc is traced out as z_1 varies so that (z_1,z_2) stays in A according to (8.70).

Recall that the circle generated by $H(t_1,t_2) = 1 - \varepsilon_3/\varepsilon^*$ is the same as that generated by $F(s_1,s_2) = 1 - \varepsilon^*/\varepsilon_3$. We will now show that a different part of the arc $C_3(z_1)$ can be attained by an actual material. An analysis similar to the one applied to $F(s_1,s_2)$ gives that the arc $C_3(z_1)$ in the H-plane can be parameterized by

$$H(t_1,t_2) = \frac{p_1}{t_1-z_1} + \frac{p_2}{t_2-z_2}, \tag{8.80}$$

where analogous to (8.70) we have

$$z_2 = \frac{b_2}{b_1} z_1 + \left(1 - a_2 - \frac{b_2}{b_1}(1 - a_1)\right) \tag{8.81}$$

Now the admissible region analogous to A in (z_1,z_2)-space for H certainly lies in the unit square. In terms of H, the condition $F(1,1) \leq 1$ translates into $H(0,0) \leq 0$, which is automatically satisfied since $0 \leq z_1,z_2 \leq 1$. However the condition that $F(0,0) \leq 0$ translates into $H(1,1) \leq 1$, so that the admissible region in (z_1,z_2)-space for H is identical to A. Thus when the line (8.81) passes through A, the section of $C_3(z_1)$ that corresponds to the line segment in A is attainable by the following geometry. Analogous to (8.79) we have

$$\varepsilon^* = \frac{1}{\dfrac{\left(1 - \dfrac{p_1}{1-z_1} - \dfrac{p_2}{z_2}\right)}{\varepsilon_3} + \dfrac{\left(\dfrac{p_1}{1-z_1}\right)}{(1-z_1)\varepsilon_1+z_1\varepsilon_3} + \dfrac{\left(\dfrac{p_2}{1-z_2}\right)}{(1-z_2)\,\varepsilon_2 + z_2\varepsilon_3}}, \qquad (8.82)$$

which is just the previous geometry rotated by 90^0. The arc is traced out as z_1 varies so that (z_1,z_2) stays in A according to (8.81). Note that the slab geometry corresponding to $\varepsilon^* = 1/(p_1/\varepsilon_1 + p_2/\varepsilon_2 + p_3/\varepsilon_3)$ or $H(t_1,t_2) = p_1/t_1 + p_2/t_2$ does not lie on the arc unless the line (8.81) passes through the origin in (z_1,z_2)-space.

A similar analysis to that above can be given to show that part of the arc of $C_1(z_1)$ can be attained by the same type of slab geometry but with the host material being ε_1. Since only parts of our bounds are attainable one expects that the bounds can be improved.

Assuming further that the material is statistically isotropic allows knowledge of F to second order as in (8.39). The G transformation then has the expansion

$$G(s_1,s_2) = \frac{p_1}{s_1} + \frac{p_2}{s_2} + \frac{p_1}{ds_1^2} + \frac{p_2}{ds_2^2} + \frac{0}{s_2 s_2} + \cdots \quad . \qquad (8.83)$$

The real Hashin-Shtrikman bounds were obtained by separately extremizing

$$G_1(s_1) = \int_0^1 \frac{\mu_1(dz_1)}{s_1-z_1} \tag{8.84}$$

and

$$G_2(s_2) = \int_0^1 \frac{\mu_2(dz_2)}{s_2-z_2} , \tag{8.85}$$

each known to second order

$$G_1(s_1) = \frac{p_1}{s_1} + \frac{p_1}{ds_1^2} + \cdots , \quad G_2(s_2) = \frac{p_2}{s_2} + \frac{p_2}{ds_2^2} + \cdots \quad . \tag{8.86}$$

Then the extremal values of G were obtained by

$$G = G_1 + G_2 . \tag{8.87}$$

To incorporate the constraints (8.86) into G_1 and G_2, we can repeat the transformation procedure developed for a single complex variable. Let

$$J_1 = \frac{1}{p_1} - \frac{1}{s_1 G_1} , \tag{8.88}$$

and similarly for G_2. Then to first order

$$J_1(s_1) = \frac{1/dp_1}{s_1} + \cdots \quad . \tag{8.89}$$

Since $J_1(s_1)$ is a function of the type (8.84), its extremal values occur when

$$J_1(s_1) = \frac{1/dp_1}{s_1-z_1}, \quad -\infty \leqslant z_1 \leqslant \infty . \tag{8.90}$$

Equivalently, G_1 is extremized when

$$G_1(s) = \frac{p_1}{s_1(1 - \frac{1/d}{s_1-z_1})}, \tag{8.91}$$

or

$$G_1(s_1) = \frac{p_1(s_1-z_1)}{s_1(s_1-z_1-1/d)}, \quad -\infty \leqslant z_1 \leqslant \infty. \tag{8.92}$$

The last expression describes a circle in the G_1-plane, and similarly for $G_2(s_2)$. The sum of these two circles

$$G(s_1,s_2) = \frac{p_1(s_1-z_1)}{s_1(s_1-z_1-\frac{1}{d})} + \frac{p_2(s_2-z_2)}{s_2(s_2-z_2-\frac{1}{d})}, \quad -\infty \leqslant z_1,z_2 \leqslant \infty \tag{8.93}$$

encloses a region R_G in the G-plane. As in the first order case above we obtain the outer circular boundary of R_G by setting

$$\arg\left(\frac{\partial G}{\partial z_1}\right) = \arg\left(\frac{\partial G}{\partial z_2}\right), \tag{8.94}$$

or

$$\arg\left(\frac{p_1/d}{s_1(s_1 - z_1 - \frac{1}{d})^2}\right) = \arg\left(\frac{p_2/d}{s_2(s_2 - z_2 - \frac{1}{d})^2}\right) . \qquad (8.95)$$

This can be satisfied if

$$\arg(s_1) + 2\arg(s_1 - z_1 - \tfrac{1}{d}) = \arg(s_2) + 2\arg(s_2 - z_2 - \tfrac{1}{d}), \qquad (8.96)$$

or

$$\tan^{-1}\left(\frac{b_2}{a_2 - z_2 - \frac{1}{d}}\right) = \tan^{-1}\left(\frac{b_1}{a_1 - z_1 - \frac{1}{d}}\right) + \frac{1}{2}\left(\tan^{-1}\left(\frac{b_1}{a_1}\right) - \tan^{-1}\left(\frac{b_2}{a_2}\right)\right). \qquad (8.97)$$

Using the rule for the tangent of a sum gives after some manipulation

$$z_2 = a_2 - 1/d + \frac{b_2(cb_1 - a_1 + 1/d) + b_2 z_1}{(b_1 + ca_1 - c/d) - cz_1} , \qquad (8.98)$$

where

$$c = \tan\frac{1}{2}\left(\tan^{-1}\left(\frac{b_1}{a_1}\right) - \tan^{-1}\left(\frac{b_2}{a_2}\right)\right). \qquad (8.99)$$

To see that the bound given by assuming second order information about G_1 and G_2 is better than the Wiener bound given by F we note the following. If G were known only to first order,

$$G(s_1,s_2) = \frac{p_1}{s_1} + \frac{p_2}{s_2} + \cdots \quad , \tag{8.100}$$

then the bound induced on F by

$$G(s_1,s_2) = \frac{p_1}{s_1-z_1} + \frac{p_2}{s_2-z_2} \tag{8.101}$$

under (8.70) is the same as in (8.65). This is so because in the 1/G-plane the circle of (8.101) becomes a horizontal line and the same holds for (8.65) in the 1/F-plane. Since

$$\frac{1}{G} = \frac{1}{F} - \frac{1}{d} , \tag{8.102}$$

the two lines are the same. Now G_1 and G_2 are known to second order, so that the bound induced by (8.86) is clearly better than that in (8.100), and consequently better than (8.65) or (8.71).

To obtain the second order bound we first apply the above considerations to $\tilde{G}(q_2,q_3)$ to obtain a region $R_{\tilde{G}}$ in the $\tilde{G}$-plane. Next we consider $H(t_1,t_2) = 1 - \varepsilon_3/\varepsilon^*$. To second order,

$$H(t_1,t_2) = \frac{p_1}{t_1} + \frac{p_2}{t_2} + \frac{\left(\frac{d-1}{d}\right)(p_1-p_1^2)}{t_1^2} + \frac{\left(\frac{d-1}{d}\right)(p_2-p_2^2)}{t_2^2} - \frac{2\left(\frac{d-1}{d}\right)p_1p_2}{t_1t_2} + \cdots \quad . \tag{8.103}$$

Then the transformation

$$L(t_1,t_2) = \frac{H}{1-\left(\frac{d-1}{d}\right)H}\ , \tag{8.104}$$

has the second order expansion

$$L(t_1,t_2) = \frac{p_1}{t_1} + \frac{p_2}{t_2} + \frac{\left(\frac{d-1}{d}\right)p_1}{t_1^2} + \frac{\left(\frac{d-1}{d}\right)p_2}{t_2^2} + \frac{0}{t_1t_2} + \cdots\ . \tag{8.105}$$

Now the same analysis can be applied to $L(t_1,t_2)$ as was applied to $G(s_1,s_2)$, yielding a region R_L in the L-plane. Finally we consider $\tilde{H}(v_2,v_3) = 1 - \varepsilon_1/\varepsilon^*$, where $v_2 = 1/(1-\varepsilon_1/\varepsilon_2)$ and $v_3 = 1/(1-\varepsilon_1/\varepsilon_3)$. The analogue of (8.104) with H replaced by $\tilde{H}$ yields a region $R_{\tilde{L}}$ in the $\tilde{L}$-plane. In the ε^*-plane we obtain four circular regions R_G^*, $R_{\tilde{G}}^*$, R_L and $R_{\tilde{L}}^*$. The second order bound is the intersection of these four regions with the first order bound.

Note that when $z_1 = z_2 = 0$ in (8.93) G attains the upper Hashin-Shtrikman bound, which we have already mentioned is realizable, at least for certain volume fractions. Only in the special case when the curve defined by (8.98) runs through $(z_1,z_2) = (0,0)$ does this geometry lie on the bound (8.93). In general the arcs defined by the above intersection violate the interchange inequality and are consequently not realizable. Thus the second order bounds can be improved.

The complex zeroth order, Wiener, and Hashin-Shtrikman bounds above are illustrated in Figure 1.

Figure 1: a. $L_{12}(\alpha)$ in (8.62)

b. $L_{23}(\alpha)$ in (8.62)

c. $C_{13}(\alpha)$ in (8.63)

d. $C_3(z_1)$ in (8.71)

e. $C_1(z_1)$ in (8.76)

f. circular boundary of R^*_G in (8.93) - (8.99)

g. circular boundary of $R^*_{\tilde{G}}$ similar to (8.93) - (8.99)

A. $\varepsilon^* = p_1\varepsilon_1 + p_2\varepsilon_2 + p_3\varepsilon_3$

B. $\varepsilon^* = 1/(p_1/\varepsilon_1 + p_2/\varepsilon_2 + p_3/\varepsilon_3)$

C. $\varepsilon^* = \varepsilon_3 + 1/(1/A_3 - 1/3\varepsilon_3)$ as in (8.55)

D. $\varepsilon^* = \varepsilon_1 + 1/(1/A_1 - 1/3\varepsilon_1)$ as in (8.55)

In Figure 1 the circular bounds of R^*_L and $R^*_{\tilde{L}}$ contain those of R^*_G and $R^*_{\tilde{G}}$ and have been omitted.

Appendix. Analytic Measures on a Discrete Torus

In section 8.B we conjectured that extremal values of a function with the representation (7.28) are attained when the measure μ is the product of a point mass with Lebesgue measure. As evidence for this conjecture, we now prove that for a discrete model of M_a in (8.19), the only extreme points are discrete versions of the measures in (8.20). In the discrete setting then the conjecture is evidently true.

Let T_N^2 be the $N \times N$ discrete torus $\{\omega^j, 1 \leq j \leq N\} \times \{\omega^k, 1 \leq k \leq N\}$, where $\omega = e^{i2\pi/N}$, and let $\hat{T}_N^2$ be the Fourier space $\{n, -(N-1) \leq n \leq N-1\} \times \{m, -(N-1) \leq m \leq N-1\}$ associated with T_N^2. Further, let M_N be the set of positive measures μ of mass 1 on T_N^2 such that their Fourier transforms $\hat{\mu}$ have no support in the interiors of the second and fourth quadrants of $\hat{T}_N^2$. This condition may be written as

$$\hat{\mu}(n,m) = \sum_{j,k=1}^{N} \mu(j,k)\, \omega^{jn+km} = 0 \ , \ mn < 0 \ , \tag{A.1}$$

where $\mu(j,k)$ is the mass of μ on the point $(j,k) \in T_N^2$. We now give a complete characterization of M_N.

<u>Definition:</u> A row measure concentrated on row k is defined by $\mu(j,k) = 1/N$, for all j.

<u>Definition:</u> A column measure concentrated on column j is defined by $\mu(j,k) = 1/N$, for all k.

<u>Theorem:</u> M_N is the convex hull of the row and column measures.

The proof of the theorem rests on the following

Lemma: For $\mu \in M_N$, $\hat{\mu}$ is supported only on the axes of $\hat{T}_N^2$.

Proof: The lemma is proved by noting that if $\hat{\mu}$ is given in the interior of one quadrant, then it is determined in the interiors of the others through complex conjugation,

$$\overline{\hat{\mu}(n,m)} = \hat{\mu}(-n, -m) \quad . \tag{A.2}$$

It is clear that if $\hat{\mu} = 0$ at (n,m), $n > 0$, $m < 0$, then $\hat{\mu} = 0$ at $(-n, -m)$ in the second quadrant, where $(-n, -m)$ is the reflection of (n,m) through $(0,0)$. However, we must note further that if $\hat{\mu} = 0$ at (n,m), $n > 0$, $m < 0$, then $\hat{\mu} = 0$ at $(-n \pmod N, -m \pmod N))$ in the first quadrant. In fact, $(-n \pmod N, -m \pmod N))$ can be interpreted as the reflection of (n,m) through the point $(N/2,0)$. For example, if $N = 5$ and $(n,m) = (3, -2)$, then $(-n, -m) = (-3, 2) = (2,2) \pmod N$. Thus $\hat{\mu}$ vanishes in the interior of each of the four quadrants of $\hat{T}_N^2$.

Before we prove the theorem, we note that if (n,m) is in the fourth quadrant, then $(-n, -m)$ can further be interpreted as being in the fourth quadrant as the reflection through $(N/2, -N/2)$. For example, if $N = 5$ and $(n,m) = (4, -2)$, then $(-n, -m) = (-4, 2) = (1, -3) \pmod N$. Thus in the fourth quadrant, off the diagonal it suffices to consider only those Fourier equations with $n > |m|$. On the diagonal it suffices to set $\hat{\mu}(1,-1) = 0$ through $\hat{\mu}(\frac{N-1}{2}, \frac{-(N-1)}{2}) = 0$ if N is odd, and through $\hat{\mu}(N/2, -N/2) = 0$ if N is even. The remaining equations are independent. Let R_{nm} be the vector in $\mathbb{C}^{N \times N}$ representing the (n,m) homogeneous Fourier equation in (A.1). Then

$$R_{nm} \cdot R_{n'm'} = \sum_{j,k=1}^{N} \omega^{j(n+n')+k(m+m')} = 0 \tag{A.3}$$

unless $n' = -n$ and $m' = -m$, so that the R_{nm} are independent.

Proof (of Theorem): Let $\hat{M}_N$ be the image of M_N under Fourier transform. We find the extreme points of $\hat{M}_N$. From the lemma and the above observations about complex conjugation, $\hat{M}_N = \{\hat{\mu}(n,0), \hat{\mu}(0,n), 1 \leq n \leq (N-1)/2\}$ if N is odd and $\hat{M}_N = \{\hat{\mu}(n,0), \hat{\mu}(0,n), 1 \leq n \leq N/2\}$ if N is even. We write this out for $N = 4$,

$$\hat{\mu}(1,0) = y_1\omega^1 + y_2\omega^2 + y_3\omega^3 + y_4\omega^4$$
$$\hat{\mu}(2,0) = y_1\omega^2 + y_2\omega^4 + y_3\omega^2 + y_4\omega^4$$
$$\tag{A.4}$$
$$\hat{\mu}(0,1) = y_5\omega^1 + y_6\omega^2 + y_7\omega^3 + y_8\omega^4$$
$$\hat{\mu}(0,2) = y_5\omega^2 + y_6\omega^4 + y_7\omega^2 + y_8\omega^4 ,$$

where $y_1,\cdots,y_4$ are the column sums $y_j = \sum_{k=1}^{N} \mu(j,k)$ and $y_{4+1}, y_{4+2},\cdots,y_{4+4}$ are the row sums $y_{N+k} = \sum_{j=1}^{N} \mu(j,k)$. Because $\hat{\mu}(1,0)$ through $\hat{\mu}(N/2,0)$ for say, N even, all involve the same y variables with just different powers of ω, we can restrict our attention to $\hat{\mu}(1,0)$. Likewise in the second set we restrict attention to $\hat{\mu}(0,1)$. We now consider the compact convex subset of $\mathbb{C}^2$, $K_N = \{(\hat{\mu}(1,0), \hat{\mu}(0,1))\}$. Finding the extreme points of K_N serves to characterize the extreme points of $\hat{M}_N$ because of the above restriction. Because the mass of a measure $\mu \in M_N$ is 1,

$$\sum_{j=1}^{N} y_j = 1 \quad , \sum_{k=1}^{N} y_{N+k} = 1. \tag{A.5}$$

Thus by (A.4) $\hat{\mu}(1,0)$ and $\hat{\mu}(0,1)$ each must lie in the convex hull W_N of the N roots of unity, which is an N-sided polygon centered about the origin in the plane. Clearly we can choose a measure in M_N so that $\hat{\mu}(1,0)$ attains any complex number in W_N. Alternatively, we can choose a measure in M_N so that $\hat{\mu}(0,1)$ attains any complex number in W_N. Consequently, any extreme point of K_N must have one of its entries equal to a vertex of W_N. Equivalently, $(z_1,z_2) \in K_N$ cannot be extreme in K_N if both z_1 and z_2 are interior points of W_N.

We see then that an extreme point of M_N is characterized by $y_j = 1$ for some j or $y_{N+k} = 1$ for some k. In order to uniquely determine these measures we study the diagonal Fourier constraints for say, N even

$$\hat{\mu}(0,0) = \sum_{j,k=1}^{N} \mu(j,k) = 1$$

$$\hat{\mu}(1,-1) = \sum_{\ell=1}^{N} x_\ell \omega^{\ell-1} = 0 \qquad \text{(A.6)}$$

$$\vdots$$

$$\hat{\mu}((N/2), -(N/2)) = \sum_{\ell=1}^{N} x_\ell \, \omega^{(N/2)(\ell-1)} = 0,$$

where x_ℓ is the sum of those $\mu(j,k)$ lying on the trajectory on T_N^2 of slope 1 which passes through $(j,k) = (\ell,1)$, $1 \leq \ell \leq N$. The mass equation $\hat{\mu}(0,0) = 1$ can be written as $\sum_{\ell=1}^{N} x_\ell = 1$. Then the system (A.6) consists of $2(N/2) + 1 = N + 1$ real equations in N unknowns with the unique solution

$$x_1 = x_2 = \cdots = x_N = 1/N. \qquad \text{(A.7)}$$

Since an extreme point μ of M_N must have $y_j = 1$ or $y_{N+k} = 1$, μ must be concentrated on one row or one column. Since there is only one trajectory of slope 1 passing through each point of a row or column (A.7) renders the mass of each point in the row or column on which μ is supported equal to 1/N. Thus the set of extreme points of M_N is precisely equal to the set of row and column measures.

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