Herglotz Functions in Inverse Homogenization
or
Recovery of Hidden Variables

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• **Classic problem: Can One Hear the Shape of a Drum**

The frequencies of vibration depend on the shape of the drum.
Given the shape, one can calculate the frequencies.

• **Mark Kac: Can one tell something about the shape if the frequencies are known?**

• Given a set of eigenvalues $\lambda_n$ of Dirichlet problem for the Laplacian for a domain $D$, what can one tell about $D$ if one knows only the values of $\lambda_n$?

• **Hermann Weyl: Area of the domain can be found from a given set of $\lambda_n$.**
• **Answers to the question about the Shape of a Drum**

Differently shaped tori have the same set of $\lambda_n$ (Milnor)

Different plane non-convex polygons have the same set of $\lambda_n$ (Gordon, Webb, Wolpert)

• **But: Both polygons have the same area and perimeter.**

• **Conclusion:** One cannot hear the shape of the drum completely (for many shapes). However, some information can be inferred.

• **Moreover, in some classes of domains (convex analytic biaxisymmetric plane regions, Zelditch) the shape can be recovered from set of $\lambda_n$.**
• **Forward Homogenization** for composite materials:

  Find the effective permittivity $\epsilon^*$. 
  Find bounds on the effective $\epsilon^*$

• **Inverse Homogenization**:

  Find microstructural information from known effective permittivity $\epsilon^*$
Homogenization of Maxwell Equations

• Time-harmonic Maxwell equations in $\varepsilon$-periodic medium

$$\begin{align*}
\nabla \times \mathbf{E}^\varepsilon(x) - i\omega\mu(x/\varepsilon)\mathbf{H}^\varepsilon(x) &= 0 \\
\nabla \times \mathbf{H}^\varepsilon(x) + i\omega\epsilon(x/\varepsilon)\mathbf{E}^\varepsilon(x) &= 0 \\
\nabla \cdot \epsilon(x/\varepsilon)\mathbf{E}^\varepsilon(x) &= 0 \\
\nabla \cdot \mu(x/\varepsilon)\mathbf{H}^\varepsilon(x) &= 0
\end{align*}$$

Here $x \in Y \subset \mathbb{R}^3$, $\mathbf{E}^\varepsilon$ and $\mathbf{H}^\varepsilon$ are electric and magnetic fields, $\epsilon$ is complex permittivity, $\mu$ is magnetic permeability.

• Let $y = x/\varepsilon \in \Omega^\varepsilon$, then $\nabla \rightarrow \nabla_x + \varepsilon^{-1}\nabla_y$, we have

$$\begin{align*}
(\nabla_x + \varepsilon^{-1}\nabla_y) \times \mathbf{E}^\varepsilon(x) - i\omega\mu(y)\mathbf{H}^\varepsilon(x) &= 0 \\
(\nabla_x + \varepsilon^{-1}\nabla_y) \times \mathbf{H}^\varepsilon(x) + i\omega\epsilon(y)\mathbf{E}^\varepsilon(x) &= 0 \\
(\nabla_x + \varepsilon^{-1}\nabla_y) \cdot \epsilon(y)\mathbf{E}^\varepsilon(x) &= 0 \\
(\nabla_x + \varepsilon^{-1}\nabla_y) \cdot \mu(y)\mathbf{H}^\varepsilon(x) &= 0.
\end{align*}$$

(N. Wellander & G. Kristensson, 2003)
Homogenization of Maxwell Equations

• Using two-scale asymptotic expansions method, we obtain homogenized Maxwell equations:

\[
\begin{align*}
\nabla \times \mathbf{E}(\mathbf{x}) - i \omega \mu^* \mathbf{H}(\mathbf{x}) &= 0, \\
\nabla \cdot \epsilon^* \mathbf{E}(\mathbf{x}) &= 0 \\
\nabla \times \mathbf{H}(\mathbf{x}) + i \omega \epsilon^* \mathbf{E}(\mathbf{x}) &= 0, \\
\nabla \cdot \mu^* \mathbf{H}(\mathbf{x}) &= 0
\end{align*}
\]

where \( \mathbf{E}, \mathbf{H} \) are the homogenized electric and magnetic fields

• \( \epsilon^* \) and \( \mu^* \) are homogenized permittivity and permeability of the medium

\[
\begin{align*}
\epsilon^* &= \langle \epsilon(\mathbf{y}) (I_3 + \nabla_{\mathbf{y}} \phi_e(\mathbf{y})) \rangle \\
\epsilon^*_{jk} &= \frac{1}{|\Omega^\epsilon|} \int_{\Omega^\epsilon} \epsilon(\mathbf{y}) \left( \delta_{jk} + \frac{\partial \phi^k_e(\mathbf{y})}{\partial y_j} \right) d\mathbf{y}
\end{align*}
\]

\[
\begin{align*}
\mu^* &= \langle \mu(\mathbf{y}) (I_3 + \nabla_{\mathbf{y}} \phi_h(\mathbf{y})) \rangle \\
\mu^*_{jk} &= \frac{1}{|\Omega^\epsilon|} \int_{\Omega^\epsilon} \mu(\mathbf{y}) \left( \delta_{jk} + \frac{\partial \phi^h_k(\mathbf{y})}{\partial y_j} \right) d\mathbf{y}
\end{align*}
\]

\( j, k = 1, 2, 3. \)

• Functions \( \phi_e \) and \( \phi_h \) are solutions of local elliptic equations:

\[
\begin{align*}
\nabla_{\mathbf{y}} \cdot \epsilon(\mathbf{y}) \nabla_{\mathbf{y}} \phi^i_e(\mathbf{y}) &= -\nabla_{\mathbf{y}} \cdot \epsilon(\mathbf{y}) \mathbf{e}_i \\
\nabla_{\mathbf{y}} \cdot \mu(\mathbf{y}) \nabla_{\mathbf{y}} \phi^i_h(\mathbf{y}) &= -\nabla_{\mathbf{y}} \cdot \mu(\mathbf{y}) \mathbf{e}_i
\end{align*}
\]
Local problem - Problem on fine scale

- Permittivity $\varepsilon$ is highly oscillating function, taking value $\varepsilon_k$ in subdomain $\Omega_k$.

$$
\varepsilon(y) = \varepsilon_1 \chi(y) + \varepsilon_2 (1 - \chi(y)), \quad y \in \Omega = \Omega^\varepsilon = \Omega_1 \cup \Omega_2
$$

$\chi(y)$ is the characteristic function of material one

$$
\chi(y) = \begin{cases} 
1, & \text{if } y \in \Omega_1, \\
0, & \text{otherwise.}
\end{cases}
$$

- Local problem for the electric potential $\phi^{(i)}$ ($i = 1, 2, 3$), $(E_i = \nabla \phi^{(i)} + e_i)$

$$
\nabla \cdot (\varepsilon_1 \chi(y) + \varepsilon_2 (1 - \chi(y))) (\nabla \phi^{(i)} + e_i) = 0, \quad y \in \Omega
$$

- The effective permittivity tensor $\varepsilon^*$ relates average displacement fields and average electric fields:

$$
< \mathbf{D} > = \varepsilon^* < \mathbf{E} >, \quad \varepsilon^* = \frac{1}{V} \int_{\Omega} \varepsilon(y) \mathbf{E}(y) \, dy
$$
Spectral representation

• We focus on one diagonal coefficient $\varepsilon^* = \varepsilon_{kk}^*$, with $E = e_k + \nabla \phi$

$$\nabla \cdot (\varepsilon_1 \chi(x) + \varepsilon_2 (1 - \chi(x))) E = 0, \quad \varepsilon^* = \langle \varepsilon E \rangle,$$

Introducing complex parameter $s$, rewrite the local problem as

$$\nabla \cdot \chi E = s \nabla \cdot E, \quad s = \frac{1}{1 - h}, \quad h = \frac{\varepsilon_1}{\varepsilon_2}.$$

Then,

$$\nabla \cdot \chi (\nabla \phi + e_k) = s \Delta \phi$$

• Introduce an operator $\Gamma = \nabla (\nabla)^{-1} (\nabla \cdot )$, and express $E$ as a function of the operator $\Gamma \chi$,

$$E = (I + \frac{1}{s} \Gamma \chi)^{-1} e_k = s (sI + \Gamma \chi)^{-1} e_k.$$
Spectral representation for $\epsilon^*$

The spectral resolution of bounded self-adjoint operator $\Gamma \chi$ with a projection valued measure $Q$ results in integral representation for $E(s)$ and $F(s) = 1 - \epsilon^*(s)/\epsilon_2$:

$$E(s) = \int_0^1 \frac{s}{s - z} dQ(z) e_k, \quad F(s) = \langle s^{-1} \chi E, e_k \rangle = \int_0^1 \frac{\langle \chi dQ(z) e_k, e_k \rangle}{s - z}$$

Let $\mu$ be a positive function of bounded variation, corresponding to the spectral measure $Q$, $d\mu(z) = \langle \chi dQ(z) e_k, e_k \rangle$, then

$$F(s) = 1 - \frac{\epsilon^*}{\epsilon_2} = \int_0^1 \frac{d\mu(z)}{s - z}, \quad s = \frac{1}{1 - \epsilon_1/\epsilon_2}.$$ 

Here $\mu$ is the spectral measure of $\Gamma \chi$.

This representation was used in homogenization to derive forward bounds on $\epsilon^*$ (Bergman’78; Milton’79; Golden-Papanicolaou’83)
Forward and Inverse Bounds

- **Forward bounds on $\epsilon^*$:**
  
  Bergman’80; Milton’80; Golden-Papanicolaou’83; Bruno’91 (Matrix-particle composites)

- **Inverse Bounds for volume fraction of one component**
  
  McPhedran, McKenzie, Milton’82; McPhedran, Milton’90; Cherkaev, Tripp’96; Cherkaev, Golden’98; Orum, Cherkaev, Golden’11
Other Approaches to Inverse Bounds

**Inverse bounds** The spectral function $\mu$ was used to derive microstructural information about the composite (Gajdardziska-Josifovska, McPhedran, McKenzie, Collins; Cherkaev, Tripp; Tripp, Cherkaev, Hulen; Cherkaev, Golden; Engstrom; Gully, Cherkaev, Golden; Orum, Cherkaev, Golden).

**Prediction of composite properties** Extract spectral function from one set of data and use it to predict properties of other composites with similar geometry or predict properties at other frequencies or temperature (Day, Thorpe; Day, Thorpe, Grant, Sievers; Osipov, Rosanov, Simonov, Starostenko).

**One measurement in inverse conductivity problem** (Ikehata; Kang, Seo, Sheen; Alessandrini, Morassi, Rosset, Seo)

**Asymptotically small volume fraction** (Ammari, Kang; Capdeboscq, Vogelius).

**Inversion of variational bounds on $\epsilon^*$** (Kang, Kim, Milton; Milton; Milton, Nquyen; Kang, Milton; Thaler, Milton).

**Parameterized multiscale inversion** (Alessandrini; C. Frederick, B. Engquist)
Integral representation for $F(s)$

The integral representation separates the parameter information in $s$ from information about the microgeometry contained in $\mu$.

$$F(s) = 1 - \frac{\epsilon^*}{\epsilon_2} = \int_0^1 \frac{d\mu(z)}{s-z}, \quad s = \frac{1}{1 - \epsilon_1/\epsilon_2}.$$

Geometric information about the microstructure is incorporated into $\mu$ via its moments, which can be calculated from the correlation functions of the medium

$$\mu_n = \int_0^1 z^n d\mu(z) = (-1)^n \langle \chi [(\Gamma \chi)^n e_k] \cdot e_k \rangle$$
Uniqueness of reconstruction of spectral measure

• **Theorem** (E.C) The measure $\mu$ can be uniquely reconstructed if the function $F(s)$ is known on an open set $C$ of the complex variable $s$ with a limiting point.

The proof is based on analytic continuation and series expansion of the integral kernel:

$$F(s) = \sum_{k=1}^{\infty} \frac{c_k}{s^k} = \sum_{n=0}^{\infty} \frac{1}{s^{n+1}} \int_0^1 z^n d\mu(z) = \frac{\mu_0}{s} + \frac{\mu_1}{s^2} + \frac{\mu_2}{s^3} + \ldots$$

The integrals are Stieltjes moments $\mu_n$ of the measure $\mu$

$$\mu_n = \int_0^1 z^n d\mu(z), \quad n = 0, 1, 2, \ldots$$

The problem of reconstruction of measure $\mu$ on the unit interval from its known moments $\{\mu_n\}$ is the Hausdorff moment problem.
**Uniqueness of reconstruction of moments**

**Theorem** (E.C - MJ.Ou) Moments of the spectral function $\mu$

$$\mu_n = \int_0^1 z^n d\mu(z) = (-1)^n \langle \chi[(\Gamma \chi)^n e_k] \cdot e_k \rangle$$

are uniquely reconstructed if the function $F(s)$ is known on an arc $S$ in the complex plane of $s$ or if effective permittivity $\epsilon^*(\omega)$ is known for a range of frequency $\omega$.

The regularized reconstruction is stable.

In particular, the zeroth moment $\mu_0$ which defines the volume fraction $f$ of one component in the composite is uniquely recovered.

$$\mu_0 = \int_0^1 d\mu(z) = \langle \chi \rangle = f$$

Analog of H.Weyl’s result for inverse spectral problem: that the area of the domain can be recovered from the set of eigenvalues.
Numerical reconstruction

- Numerical problem is ill-posed and requires regularization. The problem of reconstruction of the spectral measure $\mu$ can be reduced to an inverse potential problem: $F(s)$ admits a representation as a logarithmic potential of the measure $\mu$:

$$F(s) = \frac{\partial \Phi}{\partial s}, \quad \Phi(s) = \int_0^1 \ln |s - \lambda| \, d\mu(\lambda),$$

where $\frac{\partial}{\partial s} = \frac{\partial}{\partial x} - i \frac{\partial}{\partial y}$.

- The potential $\Phi$ solves the Poisson equation

$$-\Delta \Phi = \rho$$

where $\rho(\lambda)$ is a density on $[0, 1]$.

A solution to the forward problem is given by the Newtonian potential with $\mu(d\lambda) = \rho(\lambda) d\lambda$. The inverse problem is to find $\rho(\lambda)$ (or $\mu$) given values of $\Phi$, $\partial \Phi / \partial n$, or $\nabla \Phi$. 
Ill-posedness and regularization

- Solve the minimization problem:

\[
\min_\mu \| A\mu - F \|_2^2, \quad A\mu = \frac{\partial}{\partial s} \int_0^1 \ln |s - \lambda| \ d\mu(\lambda)
\]

with given measured data, \( F(s) = 1 - \epsilon^*(s)/\epsilon_1, \ s \in \mathbb{C} \setminus [0, 1] \).

- The problem is **ill-posed**: solution does not depend continuously on the data. Unboundedness of \( A^{-1} \) leads to arbitrarily large variations in the solution, the problem needs regularization.

- Constrained minimization regularization: augment the problem with stabilization quadratic or total variation functional which constrains the set of minimizers. Reformulate the problem as an unconstrained minimization:

\[
\min_{\mu: J(\mu) \leq \beta} A\mu - F \to \min_{\mu \in \mathcal{M}} \mathcal{J}_\alpha (\mu, F) = \| A\mu - F \|^2 + \alpha J(\mu)
\]

Regularized problem is well-posed, its solution is stable.

- Non-negativity constraint (the spectral measure of a self-adjoint operator is a non-decreasing function):

\[
\| A\mu - F \| \to \min_{\mu \in \mathcal{M}^+}
\]
Matrix measure: Uniqueness of reconstruction

- Isotropic composites: $\mu$ is a scalar measure

- Axisymmetric $\chi$ wrt spatial coords: $\mu = \text{diag}(\mu_{11}, \ldots, \mu_{dd})$ diagonalizable

- In a general case, $M = \{\mu_{ik}\}$ is a nondiagonal matrix-valued measure

\[
F(s) = I - \frac{\epsilon^*(s)}{\epsilon_1} = \int_0^1 dM(z) \frac{1}{s - z}, \quad s \in \mathbb{C} \setminus [0, 1]
\]

- **Theorem** (E.C): A determinate matrix measure $M$ can be uniquely reconstructed if the matrix function $F(s)$ is known on a open set $S$ of the complex variable $s$ with a limiting point.

A $d \times d$ positive-definite matrix of measures $M$ has moments

\[
M_n = \int_0^1 z^n dM(z), \quad n = 0, 1, 2, \ldots
\]

The measure is determinate if a problem of reconstruction of measure $M$ from its known moments $\{M_n\}$ is uniquely solvable.
Padé Approximants
Markov’s theorem for Padé approximants

- \( \{p_n\}_n \) is a sequence of polynomials orthogonal wrt \( \mu \)
- \( \{q_n\}_n \) is a sequence of polynomials of the second kind

\[
q_n(t) = \int \frac{p_n(t) - p_n(z)}{t - z} d\mu(z), \quad n \geq 0
\]

- A. Markov (1895):

\[
\lim_{n \to \infty} \frac{q_n(s)}{p_n(s)} = \int_0^1 \frac{d\mu(z)}{s - z}, \quad \text{for } s \in \mathbb{C} \setminus [0, 1]
\]

- Properties for the case of scalar \( \mu \):
  i. \( \{p_n\}_n \) is a set of polynomials orthogonal with respect to the spectral measure \( \mu \).
  ii. Zeros of orthogonal polynomials are all real, simple, and lie in the unit interval which is support of the measure \( \mu \).
Padé approximants in the scalar case

- **Diagonal Padé approximant** of order $n$ to the function $F(s)$ is a unique rational function

$$\pi_n = \frac{q_n(s)}{p_n(s)}, \quad \text{s.t.} \quad p_n(s)F(s) - q_n(s) = O\left(\frac{1}{s^{n+1}}\right).$$

where polynomial $p_n(s)$ has $\deg p_n \leq n$, and $q_n(s)$ is a polynomial part of the series $p_n(s)F(s)$. Solution to this problem always exists with $\deg p_n(s) = n$, $\deg q_n(s) \leq n - 1$.

- The rational function $\pi_n$ has a partial fraction decomposition of the form:

$$\pi_n = \frac{q_n(s)}{p_n(s)} = \sum_{j=1}^{n} \frac{r_{n,j}}{s - z_{n,j}}$$

with $r_{n,j} = \text{res}_{s=z_{n,j}} \pi_n(s) = \frac{q_n(s)}{p'(n)(s)}$, $j = 1, \ldots, n$

where $z_{n,j}$ are zeros of polynomial $p_n$, and $r_{n,j}$ are residues which are Christoffel coefficients.
Matrix-valued case

\[ F(s) = I - \frac{\epsilon^*(s)}{\epsilon_1} = \int_0^1 \frac{d M(z)}{s - z}, \quad s \in \mathbb{C} \setminus [0, 1] \]

Matrix-valued analytic function \( F(s) \) can be approximated by matrix Pade approximants.

Matrix Orthogonal Polynomials

Matrix polynomials \( P_n, P_m \) are orthogonal with respect to measure \( M \):

\[ \int_0^1 P_n(z) d M(z) P_m^*(z) = \delta_{nm} I, \quad n, m \geq 0, \quad M(z) = \{\mu_{jk}\}(z) \]

Matrix polynomials \( \{P_n\}_n \) satisfy a three-term recurrence relation:

\[ z P_n(z) = A_{n+1} P_{n+1}(z) + B_n P_n(z) + A_n^* P_{n-1}(z) \]

\[ n \geq 0, \quad P_{-1}(z) = 0, \quad P_0(z) = I \]
Generalization of Markov’s theorem

- Matrix polynomials of the second kind:
  \[ Q_n(s) = \int \frac{P_n(s) - P_n(z)}{s - z} \, dM(z), \quad n \geq 0 \]

- **Theorem** (A. Duran): For a determinate matrix measure \( M \)
  \[ \lim_{n \to \infty} P_n^{-1}(s) Q_n(s) = \int_0^1 \frac{dM(z)}{s - z}, \quad \text{for} \quad s \in \mathbb{C} \setminus [0, 1] \]
  Convergence is uniform for \( s \) in compact subsets of \( \mathbb{C} \setminus [0, 1] \).

- For given \( \{P_n\}_n \), the corresponding measure can be found as weak accumulation points of a sequence of discrete measures with support in a set of zeros of \( \{P_n\} \)
  \[ \mu_n = \sum_{k=1}^m \delta_{z_{n,k}} G_{n,k} \]
Matrix Orthogonal Polynomials

• Let $z_{nk}$ be zeros of $P_n(z)$ (in increasing order) of multiplicity $l_k$

• Let $G_{nk}$ be matrices:

$$G_{nk} = \frac{1}{\det(P_n(z))^{l_k}(z_{nk})} \left( Adj(P_n(z)) \right)^{l_k-1}(z_{nk}) Q_n(z_{nk})$$

• If $l_k = 1$:

$$G_{nk} = \frac{Adj(P_n(z))(z_{nk}) Q_n(z_{nk})}{(det(P_n(z)))'(z_{nk})}$$

• Matrix Padé approximation can be written as:

$$P_{n}^{-1}(s) Q_{n}(s) = \sum_{k=1}^{m} G_{nk} \frac{1}{s - z_{nk}}$$

where $m$ is the number of zeros of $P_n(z)$.
Moments of matrix-valued measure

- Quadrature formula for matrix polynomials:
  For any matrix polynomial $P(z)$ of degree $\deg(P) \leq 2n - 1$:
  \[
  \int_0^1 P(z) \, dM(z) = \sum_{j=1}^{m} P(z_{nj})G_{nj}
  \]
  In particular, moments of the matrix-valued measure are exactly calculated for $k \leq 2n - 1$

- The moments $M_k$ of the matrix-valued spectral measure $M$
  of the operator $\Gamma \chi = \nabla (-\Delta)^{-1} (\nabla \cdot \chi)$ are given by
  \[
  M_k = \sum_{j=1}^{m} G_{nj} z_{nj}^k
  \]
  These formulas are exact for $k = 0, 1, \ldots, 2n - 1$. 
Matrix Padé Approximation

Matrix Padé approximant to the matrix-valued function \( F(s) \) is a solution of the following optimization problem:

- Find a matrix rational function \( R(s) \), \( \text{deg}(R) \leq n \),

\[
R(s) = \sum_{j=1}^{m} G_{n,j} \frac{1}{s - z_{n,j}}
\]

- such that

\[
||F(s) - R(s)||_{L^2(S)} \rightarrow \text{min},
\]

- subject to the following constraints:

\[
0 \leq s_{n,j} \leq 1,
\]

\( G_{n,j} \) are positive-semidefinite
Padé Approximants

(a-b) Reconstructed spectral density functions $m(x)$ for 2D Bruggeman model of Mg-MgF$_2$ composite with magnesium (Mg) volume fractions (a). $f = 0.2$ and (b) $f = 0.85$.

(c) True and computed spectral measure $\mu(x)$ for 85% Mg-15% MgF$_2$ composite using Padé approximation of different orders.

A pole at the origin corresponds to the volume fraction of conducting component above percolation threshold $f = 0.85$. 

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Applications

- Polycrystalline Composites: Sea Ice
- Viscoelastic Composite Material: Bone
- Hidden (Internal) Variables
Sea Ice is a Polycrystalline Composite

- Cross-polarized images of different crystalline structure of sea ice
- Top: Columnar sea ice has crystals predominantly oriented in the vertical direction
- Bottom Left: Platelet ice from the Ross Sea.
  Right: Granular ice from the Bellingshausen Sea.
- Granular ice is a statistically isotropic polycrystalline composite material.
Polycrystalline Composites

In a polycrystalline material each crystal has the same complex permittivity tensor $\varepsilon$ with different orientation.

- G. Milton, 1982;
- S. Barabash, D. Stroud, 1999;
- B. Murphy, E. Cherkaev, K. Golden, 2016;
Polycrystal

In a polycrystalline material each crystal has the same complex permittivity tensor $\varepsilon$ with different orientation given by a rotation matrix $B(x)$. For transversely isotropic or uniaxial $\varepsilon$:

$$
\varepsilon = \begin{bmatrix}
\varepsilon_1 & 0 & 0 \\
0 & \varepsilon_2 & 0 \\
0 & 0 & \varepsilon_2
\end{bmatrix}, \quad \varepsilon(x) = B^{-1}(x) \varepsilon B(x)
$$

The effective $\varepsilon^*$ has components: $[\varepsilon^*]_{jk} = e_j^T \varepsilon^* e_k = \langle e_j^T \varepsilon E_k \rangle = \langle e_j^T B^{-1} \varepsilon B E_k \rangle$.

Introduce $h = \varepsilon_1/\varepsilon_2$, $s = 1/(1-h)$ and matrices $C = e_1(e_1)^T$ and $R = B^{-1}CB$.

$$
m_{jk}(h) = \frac{\varepsilon^*_{jk}}{\varepsilon_2} = \langle e_j^T B^{-1} \begin{bmatrix} h & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} B E_k \rangle = \langle e_j^T (I - (1-h)B^{-1}CB) E_k \rangle
$$

$$
m_{jk}(h) = \langle e_j^T (I - (1-h)R) E_k \rangle \quad \text{and} \quad F_{jk}(s) = 1 - m_{jk}(h) = 1 - \frac{\varepsilon^*_{jk}}{\varepsilon_2} = \langle (s^{-1}e_j^T R) E_k \rangle
$$
Polycrystal: Resolvent representation of $\epsilon^*$

A resolvent representation for $E$ leads to an integral representation for $F(s)$.

Fluctuations $G$ in the electric field, $E_k = e_k + G$, may be represented as solution of

$$\nabla \cdot (I - s^{-1} R)(e_k + G) = 0,$$

which results in the equation $sG + \nabla(-\Delta)^{-1} \nabla \cdot (R E_k) = 0$. Introducing an operator $\Gamma = \nabla(-\Delta)^{-1} \nabla \cdot$ projecting fields onto a subspace of curl-free mean-zero fields, gives the resolvent representation for $E$:

$$E_k = s[sI + \Gamma R]^{-1} e_k.$$

This allows to express $F_{jk}(s)$ as $F_{jk}(s) = \langle e_j^T R [sI + \Gamma R]^{-1} e_k \rangle$. Applying the spectral theorem results in a representation for $F(s)$ as:

$$F_{jk}(s) = \int_0^1 \frac{d\mu_{jk}(z)}{s - z},$$

where the positive-definite matrix-valued measure $M = \{\mu_{jk}\}$ on $[0, 1]$ is the spectral measure of the self-adjoint operator $\Gamma R = \nabla(-\Delta)^{-1} \nabla \cdot R$ with $R = B^{-1} C B$ and $C = e_1(e_1)^T$. 

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Characterization of Bone Structure

Left: Normal bone. Right: Osteoporotic bone, which is more porous, weaker and subject to fracture.
Herglotz Function: Viscoelasticity

Elastic composites:
Kantor, Bergman’84,’86; Bruno, Leo’93; Milton’02; Ou, Cherkaev’06; Ou’07

Viscoelastic torsion: Tokarzhevsky, Telega, Galka’01; Bonifasi-Lista, Cherkaev’06,’08

Viscoelastic (different viscoelastic shear, same elastic bulk):
Cherkaev, Bonifasi-Lista’11

Elastic (viscoelastic) 2 parameters: Ou’11
Viscoelastic Problem

- Assumptions: the constituents are isotropic materials with the same elastic bulk modulus $\kappa$, and different shear moduli: viscoelastic $\mu_1(\omega)$, elastic $\mu_2$.

- $\Omega = \Omega_1 \cup \Omega_2$: viscoelastic phase $C^1$ is in $\Omega_1$, elastic phase $C^2$ fills $\Omega_2$.

BPV for displacement $u$:

$$
\sigma_{ij,j} = 0, \quad \sigma_{ij} = C_{ijkl}\epsilon_{kl} \quad \text{in} \quad \Omega, \quad u_i = \epsilon_{ij}^0 x_j \quad \text{on} \quad \partial \Omega.
$$

Here $\epsilon$ and $\sigma$ are tensors of strain and stress, $\epsilon = \nabla^s u = (\nabla u + \nabla u^T)/2$.

- The fourth order stiffness tensor $C$ is

$$
C(x) = \chi(x)C^1 + (1 - \chi(x))C^2.
$$

The effective viscoelastic tensor $C^*$ is a coefficient of proportionality between the average strain $<\epsilon>$ and stress, $<\sigma>$:

$$
< \sigma_{ij} > = \frac{1}{|\Omega|} \int_{\Omega} \sigma_{ij}(x)dV = C_{ijkl}^* \epsilon_{kl}^0 = C^* : \epsilon^0.
$$
Viscoelastic problem

- Introduce hydrostatic $\Lambda_h$ and deviatoric $\Lambda_s$ projections:

\[
\{\Lambda_h\}_{ijkl} = \delta_{ij}\delta_{kl}, \quad \{\Lambda_s\}_{ijkl} = \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}.
\]

$\Lambda_h$ and $\Lambda_s$ are isotropic fourth order tensors projecting onto the orthogonal subspaces of the second order tensors comprised of tensors proportional to the identity tensor and trace-free tensors.

Then, $C^i = \kappa \Lambda_h + \mu_i \Lambda_s$, $i = 1, 2$, and the BVP takes the form:

\[
\nabla \cdot (\kappa \Lambda_h + (\mu_1 \chi(x) + (1 - \chi(x))\mu_2)\Lambda_s) : \epsilon = 0
\]

- **Theorem** (E.C - C.Bonifasi-Lista) Integral representation of $C^*$

\[
F(s) = \frac{\epsilon^0 : C^2 : \epsilon^0 - \epsilon^0 : C^* : \epsilon^0}{\epsilon_s^0 : C^2 : \epsilon_s^0} = \int_0^1 \frac{d\eta(z)}{s - z}
\]

where $d\eta(z) = \langle dQ(z)e_s, e_s \rangle$ is the spectral measure of $\Lambda_s G \chi \Lambda_s$

$e_s$ is a unit strain tensor: $e_s = \Lambda_s : \epsilon^0 / ||\Lambda_s : \epsilon^0||$ and $\epsilon_s^0 = \Lambda_s : \epsilon^0$
Reconstructed spectral function for bone samples

Figure 1: (a) Bone sample. (b) Spectral functions reconstructed using Tikhonov regularization for the samples of old bone and young bone. (c) Moments of the spectral function of the bone structure (+) and of Maxwell-Garnett composite (*) of the same porous volume.
Viscoelastic medium

- The stress $\sigma$ and strain $\varepsilon$ in a linear viscoelastic medium are related by

$$\sigma = G \ast d\varepsilon = \int_{-\infty}^{t} G(t - \tau)d\varepsilon(\tau),$$

where $G(t)$ is the relaxation function of the medium.

- Fourier transform: $\sigma(\omega) = M(\omega)\varepsilon(\omega)$ with viscoelastic modulus $M$

$$M(\omega) = M_0 - \delta M \int_0^\infty \frac{d\eta(x)}{i\omega + x}$$

where $d\eta(x) = \Phi(-\ln x)dx$, $\Phi(\ln\tau)$ is the normalized relaxation spectrum of the medium with the relaxation time $\tau = x^{-1}$.

$$M_0 = M_U = \lim_{\omega \to \infty} M(\omega), \quad M_R = \lim_{\omega \to 0} M(\omega), \quad \delta M = M_0 - M_R.$$ 

- For a complex variable $\lambda = i\omega$, $G(\lambda)$ is a Stieltjes function

$$G(\lambda) = \frac{M_0 - M(\lambda/i)}{\delta M} = \int_0^\infty \frac{d\eta(x)}{\lambda + x}, \quad \lambda \in \mathbb{C} \setminus (-\infty, 0)$$

with the non-negative measure $\eta$ on $[0, \infty)$. 

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Pade approximation and internal variables

Pade approximation of $G(\lambda)$

$$G(\lambda) \approx \sum_{n=1}^{q} \frac{A_n}{\lambda - \rho_n}, \quad A_n > 0, \quad -\infty < \rho_n < 0$$

results in equations for internal memory variables $\zeta_n(t)$.

$$\sigma(t) = M_0 \left[ \varepsilon(t) - \sum_{n=1}^{q} \zeta_n(t) \right] = M_0 \varepsilon(t) - M_0 \sum_{n=1}^{q} \zeta_n(t)$$

- The **elastic** part $\sigma_e$ of the stress (instantaneous response): $\sigma_e(t) = M_0 \varepsilon(t)$
- An **anelastic** part $\sigma_d$ of the stress is:

  $$\sigma_d(t) = M_0 \sum_{n=1}^{q} \zeta_n(t)$$

- Functions $\zeta_n(t)$ are **internal memory variables** satisfying

  $$\frac{d\zeta_n(t)}{dt} = \rho_n \zeta_n(t) + A_n \frac{\delta M}{M_0} \varepsilon(t), \quad n = 1, 2, \ldots, q$$
Internal variables and spectral measure of composites

- Evolution of the internal variables $\zeta_n(t)$ is governed by the system of DEs:
  \[
  \frac{d\zeta_n(t)}{dt} = \rho_n \zeta_n(t) + A_n \frac{\delta M}{M_0} \varepsilon(t), \quad n = 1, 2, \ldots, q
  \]

- **Theorem** The coefficients $A_n$ and $\rho_n$ of the system of DEs governing the evolution of the internal variables $\zeta_n(t)$ are poles $s_{q,n}$ and residues $r_{q,n}$ of Pade approximant of the spectral measure of the composite, conformally mapped onto the complex $\lambda$-plane.

- Poles and residues of Pade approximant of the spectral measure correspond to the **exact moments** of the measure.

- In some classes of composite structures, there is a unique correspondence between the spectral measures and the geometries.

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