Padé Approximations in Inverse Homogenization and Numerical Simulation of Electromagnetic Fields in Composites

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***Abstract*—The paper considers rational Padé approximation of the spectral function of composites with fine microstructure and discusses its use in characterization of the microgeometry of composite materials and in numerical simulation of time-domain electromagnetic fields in composites. It is assumed that the scale of the structure is much smaller than the smallest wavelength of the applied field. We use Stieltjes representation of the effective complex permittivity of the composite and derive its Padé approximation. The spectral function in this representation contains all information about the microgeometry of the mixture. Having reconstructed the Padé approximation, we recover information about the composite structure. The resulting time-domain equations governing the electromagnetic fields are of convolution type. We use rational Padé approximation to derive equations for internal variables for time-domain simulation. We show that electromagnetic fields computed using such internal variables, correspond to the fields in S-equivalent composite structures.**

I. Introduction

Inverse homogenization problem is a problem of extracting information about the microstructure of composite from effective or homogenized measurements. Microstructural characterization of composite materials is an important in various applications problem [14], [4], [12], [3], [17]. The paper discusses Padé approximations for extraction of geometric information about the structure of two-phase composite medium from the effective complex permittivity and numerical simulation of time-domain electromagnetic fields in composites. The approach is based on reconstruction of the spectral measure [5] in the Stieltjes analytic representation of the effective complex permittivity ϵ^* developed in the course of computing bounds for ϵ^* of a two-component composite obtained from materials with permittivity ϵ_1 and ϵ_2 [2],[15],[13]. The spectral measure in this analytic representation contains information about the microgeometry of the composite. It is shown in [5] that the measure μ can be uniquely recovered from the effective complex permittivity given on an arc $\mathcal{C} \subset C$ in the complex plane: $\epsilon^*(s), s \in \mathcal{C}$.

Padé approximations of order $[p, q]$ are introduced for approximation of the spectral function in [17], [18] and used for estimation of volume fractions of the constituents in the composite. Diagonal Padé approximants for inverse homogenization are suggested in [6], where the analytic integral representation for ϵ^* is viewed as representation for Markov function, and properties of diagonal Padé approximants to Markov function are used to formulate the problem as a best approximation problem. The suggested method of construction of diagonal Padé approximants [6] is based on solution of constrained optimization problem. The optimization problem seeks to find a rational function of prescribed degree which minimizes distance to the given function of effective permittivity. The introduced constraints for the zeros of the denominator polynomials and residues of the corresponding partial fraction decompositions stem from the properties of Padé approximants. Using diagonal Padé approximations, the moments μ_k of the spectral measure μ are calculated exactly for $k \leq 2n-1$ [6]. We pursue this approach here.

The constructed Padé approximation can be used to extract microstructural information or to estimate other effective properties of the same composite [7]. It can also be used to derive equations for internal variables in time-domain simulations, moreover, using n-th order Padé approximation is equivalent to propagation of electromagnetic field in S_N- equivalent medium with $N = 2n-1$. Microstructures of composites which cannot be distinguished by effective measurements are $S - equivalent$ structures [5], they correspond to the same spectral functions. We define structures as $S_N - equivalent$, if the first N moments of their spectral measures are the same. If two different structures have effective permittivities with the same Padé approximations of order n, then they have $2n-1$ moments coinciding on the complex plane, so the structures are S_N- equivalent with $N = 2n-1$.

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II. Analytic representation of the effective property

The Stieltjes analytic representation for the function $F(s) = 1 - \epsilon^*(s)/\epsilon_2$ has the following form ([2], [15], [13]):

$$F(s) = \int_0^1 \frac{d\mu(z)}{s - z}\,, \qquad s = \frac{1}{1 - \epsilon_1/\epsilon_2} \tag{1}$$

where the positive measure μ is the spectral measure of a self-adjoint operator $\Gamma\chi$, $\Gamma = \nabla(-\Delta)^{-1}(\nabla\cdot)$, and $(-\Delta)$ is the Laplacian operator, and χ is the characteristic function of the domain occupied by the first material.

The spectral measure μ contains all information about the function χ and about the structure of the medium; having reconstructed it, we recover information about the structure χ. It was shown in [5] that the measure μ can be uniquely reconstructed if the function $F(s)$ is known on an open set $\mathcal{C} \subset \mathbf{C}$ of the complex variable s with a limiting point. The proof of this theorem is based on analytic continuation and reduction of the problem to Hausdorff moment problem. From this result it follows immediately that the moments μ_n of the measure μ can be uniquely recovered under the same conditions.

III. Padé approximants to Markov function $F(s)$

A. Diagonal Padé approximants

The integral representation (1) of $F(s)$ shows that function $F(s)$ is Markov function of the measure μ. Suggested in [6] approach to Padé approximations exploits this fact and is based on a number of special properties of Padé approximants to Markov functions. Diagonal Padé approximant of order n to the function $F(s)$ is a unique rational function π_n

$$\pi_n = \frac{P_n(s)}{Q_n(s)}, \quad \text{s.t.} \quad Q_n(s)F(s) - P_n(s) = O\left(\frac{1}{s^{n+1}}\right) \tag{2}$$

where polynomial $Q_n(s)$ has $\deg Q_n \le n$, and $P_n(s)$ is a polynomial part of the series $Q_n(s)F(s)$. It is known that the solution to this problem always exists with $\deg\ Q_n(s) = n, \deg\ P_n(s) \le n-1$.

It can be shown that $\{Q_n\}$ is a set of polynomials orthogonal with respect to the spectral measure μ, and zeros of orthogonal polynomials are all real, simple, and lie in the convex hull $\hat{S_\mu}$ of support of the measure μ. Then the rational function π_n has a partial fraction decomposition of the form:

$$\pi_n = \frac{P_n(s)}{Q_n(s)} = \sum_{j=1}^{n} \frac{r_{n,j}}{s - s_{n,j}} \tag{3}$$

$$\text{with} \quad r_{n,j} = res_{s=s_{n,j}} \pi_n(s) = \frac{P_n(s)}{Q\prime_n(s)}, \quad j = 1, ..., n \tag{4}$$

where $s_{n,j}$ are zeros of polynomial Q_n, and $r_{n,j}$ are residues which are Christoffel coefficients.

We show in [8] that the diagonal Padé approximation to the function $F(s)$ is a solution of the optimization problem. Diagonal Padé approximant $\pi_n(s)$ to the Markov function $F(s)$ solves the following optimization problem: Find a rational function

$$r(s) = \frac{P_n(s)}{Q_n(s)}, \quad \deg\ r \le n \tag{5}$$

such that

$$||F(s) - r(s)|| \to \min \tag{6}$$

subject to the following constraints:

$$0 \le s_{n,j} \le 1, \quad 0 \le r_{n,j} \le 1\,. \tag{7}$$

Proof is based on Gauss-Jacobi formula and the fact that the support of the measure μ in the representation (1) belongs to the unit interval, $\hat{S_\mu} \in [0,1]$. Convergence of the sequence of Padé approximants to the Markov function is known, it is given by Markov theorem.

B. Numerical algorithm

This justifies the numerical approach suggested in [18] for constructing Padé approximations for the spectral function. This method can be summarized in the following way. The real coefficients a_i and b_j of two polynomials $P(s)$ and $Q(s)$ of orders p and q are found from solution of problem of approximation of the known values of the function $F(s)$. The Padé approximation of $F(s)$ (see [1]) is:

$$F(s) \simeq F_{[p,\ q]}(s) = \frac{P(s)}{Q(s)} = \frac{a_0 + a_1 s + a_2 s^2 + \cdots + a_p s^p}{b_0 + b_1 s + b_2 s^2 + \cdots + b_q s^q} \tag{8}$$

Given measured data pairs (t_k, f_k) $(k = 1, 2, \ldots, N)$, with f_k being the measured value of the function $F(s)$ at the sample point t_k, $f_k = F(t_k)$, and with N being the total number of data points, we look for the coefficients a_i and b_j so that the functions in (8) agree in the points t_k $(k = 1, 2, \ldots, N)$. We assume that the function $F(s)$ has at least one pole (otherwise, it is zero), and use a nonstandard normalization of the polynomial coefficient $b_1 = 1$ in the denominator $Q(s)$ so that the rational function in (8) at the sample point t_k has the form:

$$\frac{a_0 + a_1 t_k + a_2 t_k^2 + \cdots + a_p t_k^p}{b_0 + t_k + b_2 t_k^2 + \cdots + b_q t_k^q} \tag{9}$$

where a_i $(i = 0, \ldots, p)$, b_j $(j = 0, \ldots, q, j \ne 1)$ are required unknown coefficients. We prove [8] the existence of Padé approximants with this nonstandard normalization for the coefficient $b_1 = 1$.

Theorem 1 The coefficient b_1 in the denominator $Q(s)$ of the Padé approximation of the spectral function $F(s)$ does not turn to zero, hence an approximation (8) of the function $F(s)$ always exists for normalization $b_1 = 1$.

Indeed, if s_k $(k = 1, \ldots, q)$ are the poles of the denominator polynomial $Q(s)$ in (8), then by Vieta theorem, the coefficients b_k/b_q $(k = 0, ..., q)$ in the denominator $Q(s)$ are:

$$\begin{cases} b_0/b_q = (-1)^q s_1 s_2 \ldots s_q \\ b_1/b_q = (-1)^{q-1}(s_1 s_2 \ldots s_{q-1} + \cdots + s_2 s_3 \ldots s_q) \\ \ldots\ldots \\ b_{q-1}/b_q = -(s_1 + s_2 + \cdots + s_q), \quad b_q/b_q = 1. \end{cases} \tag{10}$$

The roots of $Q(s)$ are simple, distinct, and are located in the unit interval (as the roots of polynomials orthogonal with respect to measure μ): $0 \leq s_1 < s_2 < \cdots < s_q < 1$. Hence, all the coefficients b_k $(k = 0, 1, ..., q)$ are non-zero except possibly b_0 which can turn to zero if $s_1 = 0$. Therefore, Padé approximation (8) of the function $F(s)$ always exists for the normalized coefficient $b_1 = 1$.

We notice that since the coefficient b_0 can turn to zero if $s_1 = 0$, the standard normalization for Padé approximation with $b_0 = 1$ is not applicable here.

C. Moments of the function μ

Using Laurent expansion of the function $F(s)$ and expanding the integral Cauchy kernel, we obtain a series representation for $F(s)$ with the coefficients given by Stieltjes moments μ_k of the measure μ

$$F(s) = \sum_{k=0}^{\infty} \frac{1}{s^{k+1}} \int_0^1 z^k d\mu(z) \; = \sum_{k=0}^{\infty} \frac{\mu_k}{s^{k+1}}, \qquad (11)$$

$$\mu_k = \int_0^1 z^k d\mu(z)\,, \qquad k = 0, 1, 2, ... \qquad (12)$$

Accuracy of diagonal Padé approximation is: $F(s) - \pi_n(s) = O\left(s^{-(2n+1)}\right)$. Expanding the partial fraction (3) into series, and comparing with power series expansion of $F(s)$, it was shown in [6] that

Theorem 2 The formulas for the moments μ_k of the spectral measure μ of operator $\Gamma\chi = \nabla(-\Delta)^{-1}(\nabla \cdot \chi)$ are given by

$$\mu_k = \sum_{j=1}^{n} r_{n,j} s_{n,j}^k\,. \qquad (13)$$

These formulas are exact for $k = 0, 1, ..., 2n - 1$.

IV. S-EQUIVALENCE OF COMPOSITE STRUCTURES

There can exist many microgeometries that generate the same effective complex permittivity measurements (the same response under the applied fields) for any materials filling in the geometric structures. It is shown in [16] that in 2D, there is a unique correspondence between the set of the spectral functions μ and the set of sequentially layered laminated materials. Theoretically, even if we can determine the microstructure of the mixture from the given measurements of the complex permittivity in a continuous interval of the values of the pure materials, this determination is probably non-unique. In this case, different composite materials could have the same effective complex permittivity for the same phase components in the mixtures.

A new concept of the S-equivalency of structures was introduced in [5], presenting classes of microstructures equivalent from the spectral measure point of view. Given two composites with the effective properties ϵ^{*_i}, $i = 1,\ 2$, and the permittivity of the pure materials ϵ_j, $j = 1,\ 2$, we say that their microstructures are S-different, if there exist $\tilde{\epsilon_j} \in \mathbf{C}$, $j = 1,\ 2$, such that $\epsilon^{*_1}(\tilde{\epsilon_1}, \tilde{\epsilon_2}) \neq \epsilon^{*_2}(\tilde{\epsilon_1}, \tilde{\epsilon_2})$. Otherwise, these two structures are S-equivalent.

From this definition, the S-equivalence of two structures implies that they have the same effective permittivity $\epsilon^{*_i}, i = 1, 2$ in any range of frequency. It turns out that the corresponding spectral functions $F^i(s), i = 1, 2$, coincide for any $s \in \mathbf{C}$ in the complex s-plane. On the contrary, for S-different structures, there exists a point $\tilde{s} \in \mathbf{C}$ such that $F^1(\tilde{s}) \neq F^2(\tilde{s})$. Using analyticity of the functions F^i, it is seen that the S-different structures correspond to different spectral functions μ. If the function $F(s)$ is known on an arc $\mathbf{C}$ in the complex s-plane, the microgeometries of different mixtures are distinguishable by the effective measurements up to the S-equivalence of structures. In other words, different microgeometries corresponding to the same spectral measure $\mu(z)$ are S-equivalent structures that can not be distinguished by effective measurements, and moreover, they are characterized by the same moments μ_k, $k = 0, 1, ...$, of the spectral function μ.

Aiming at developing an efficient method of finite difference computation of propagation of electromagnetic fields in composites, we introduce S_N-equivalent structures [9] as microgeometries of composites that are characterized by the same N moments μ_k, $k = 0, 1, ..., N$, of the spectral function μ. From Theorem 2, we have the following characterization of S_N-equivalent structures. If two different structures have Stieltjes functions $F(s)$ with the same Padé approximation of order n, then they have $2n - 1$ moments coinciding on the complex plane, so the structures are S_N- equivalent with $N = 2n - 1$.

Theorem 3 Stieltjes functions $F^i(s), i = 1, 2$, of S_N-equivalent microstructures have the same Padé approximations of order n, with $N = 2n - 1$, and hence their difference is of order $O\left(s^{-(2n+1)}\right)$.

Finite difference time domain calculations of propagation of electromagnetic, acoustic and seismic fields in dissipative conducting or viscoelastic materials often use Padé approximations for constructing internal variables in the computational scheme [10],[11],[19]. Low order Padé approximations allow to design effective numerical algorithms. Since n-th order Padé approximant corresponds to a S_N-equivalent structure, the use of internal variables in such numerical algorithms designed for computation of the fields' propagation in composite materials, is equivalent to simulation of the fields using the corresponding S_N-equivalent composite structure, with $N = 2n - 1$.

V. NUMERICAL SIMULATIONS

To show results of numerical reconstruction of spectral density function, we consider an isotropic mixture of magnesium (Mg) in magnesium fluoride (MgF_2) and compute frequency–dependent effective permittivity using 2D or 3D Bruggeman effective medium approximation [20] ($f_c = 1/3$):

$$F(s) = \frac{3(f - f_c)\, H(f - f_c)}{2s} + \int_0^1 \frac{m(x)\mathrm{d}x}{s - x}, \qquad (14)$$

where H is Heaviside function, f is volume fraction of the first material, and the spectral density function is $m(x) = \sqrt{-9x^2 + 6(f + 1)x - (3f - 1)^2}/(4\pi x)$ if $x_1 < x < x_2$,

$m(x) = 0$ for $x \leq x_1$ or $x \geq x_2$, and $x_{1,2} = (f + 1 \pm (8f(1-f))^{1/2})/3,\ 0 \leq x_1 < x_2 < 1$.

The permittivity of magnesium fluoride ($\mathrm{MgF_2}$) taken as the background matrix material in the mixture, is a dispersionless constant, $\epsilon_1 = 1.96$. The frequency–dependent permittivity of the metallic particles of magnesium (Mg) considered as inclusion material in the composite, is given by the Drude dielectric model

$$\epsilon_{\mathrm{metal}}(\omega) = 1 - \frac{\omega_{\mathrm{p}}^2}{\omega(\omega + \mathrm{i}\gamma)} \tag{15}$$

where ω is the circular frequency, ω_{p} is the plasma frequency, $\omega_{\mathrm{p}} = 9.4 \times 10^{15}\mathrm{s}^{-1}$, and γ is the damping constant, with $\tau = 1/\gamma = 2.5 \times 10^{-16}\mathrm{s}$.

We used the simulated in frequency domain effective permittivity of Bruggeman composite [20] as data for the developed algorithm. The reconstructed spectral density function $m(x)$ for $\mathrm{MgMgF_2}$ composite with magnesium volume fraction $f = 0.85$ for 2D Bruggeman model of the composite, is shown in Fig. 1. Results of reconstruction of the moments of the spectral function for 3D Bruggeman model of the composite with magnesium volume fraction $f = 0.2$ were compared with results of numerical integration of the spectral function. Moments calculated using (13) with $n = 8$ are $\mu_0 = 0.199999995$, $\mu_1 = 0.053333352$, $\mu_2 = 0.021333310$, $\mu_3 = 0.010429627$. The same moments calculated with trapezoidal rule are $\mu_0 = 0.199999985$, $\mu_1 = 0.053333332$, $\mu_2 = 0.021333333$, $\mu_3 = 0.010429629$. The numerical results show excellent agreement of theoretical and predicted values.

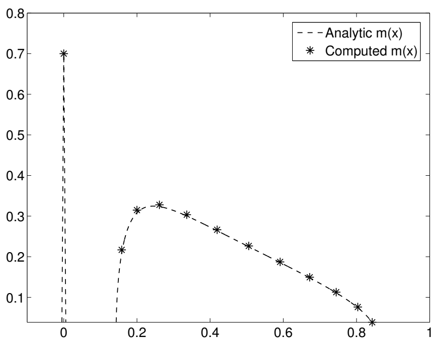

Fig. 1. 2D Bruggeman model: Reconstructed spectral density function $m(x)$

VI. Conclusion

The paper discusses the problem of characterization of microstructure of composite media using diagonal Padé approximants. The developed algorithm of Padé approximation is based on constrained least squares optimization with the constraints providing regularization of the problem. We formulate the problem as a best approximation problem, show existence of Padé approximants with the introduced normalization, discuss relation to the polynomials orthogonal with respect to the spectral measure. We use the developed Padé representation for calculation of the moments of the spectral function, the moments contain all structural information about the microgeometry of the composite. We also discuss the S-equivalent composite microstructures and application of Padé approximants and S-equivalency in finite difference numerical simulation of propagation of electromagnetic fields in composites.

Acknowledgment

This work was supported by NSF grants DMS-0508901 and DMS/CMG-0934721. The second author is funded by a Postdoctoral Fellowship at the University of Calgary.

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