Strong–Property–Fluctuation Theory for Homogenization of Bianisotropic Composites

T.G. Mackay[1], A. Lakhtakia[2], and W.S. Weiglhofer[1]

[1] Department of Mathematics, University of Glasgow
University Gardens, Glasgow G12 8QW, Great Britain
Fax: + 44 141 330 4111; email: tm@maths.gla.ac.uk

[2] CATMAS — Computational & Theoretical Materials Sciences Group
Department of Engineering Science and Mechanics, Pennsylvania State University
University Park, PA 16802–6812, USA

Abstract

The strong–property–fluctuation theory (SPFT) is developed for the homogenization of bianisotropic composites with two constituent material phases. A bianisotropic comparison medium is introduced as an initial ansatz in the perturbative process resulting in the SPFT estimate of the constitutive properties of the homogenized medium. Analytic results are presented for ellipsoidal topology, and under the bilocal and long–wavelength approximations.

1. Introduction

Many homogenization approaches — exemplified by the Maxwell Garnett and the Bruggeman formalisms, and their variants — are limited through their simplistic treatments of the distributional statistics of the constituent material phases [1]. A notable exception is the strong–property–fluctuation theory (SPFT), which provides a method to determine both local and nonlocal constitutive properties of composites while allowing for a sophisticated handling of the distributional statistics [2]. The theory has already been developed for isotropic dielectric [2], anisotropic dielectric [3], as well as chiral–in–chiral composites [4]. We present here a generalization of the theory to bianisotropic mediums; further details are reported elsewhere [5].

2. SPFT Preliminaries

We begin with the constitutive relations of a nonhomogeneous bianisotropic medium[1]

$$\underline{D}(\underline{r}) = \underline{\underline{\epsilon}}(\underline{r}) \cdot \underline{E}(\underline{r}) + \underline{\underline{\xi}}(\underline{r}) \cdot \underline{H}(\underline{r}) \,, \qquad \underline{B}(\underline{r}) = \underline{\underline{\zeta}}(\underline{r}) \cdot \underline{E}(\underline{r}) + \underline{\underline{\mu}}(\underline{r}) \cdot \underline{H}(\underline{r}) \,, \tag{1}$$

where $\underline{\underline{\epsilon}}(\underline{r})$ and $\underline{\underline{\mu}}(\underline{r})$ are the permittivity and permeability dyadics, respectively, and $\underline{\underline{\xi}}(\underline{r})$ and $\underline{\underline{\zeta}}(\underline{r})$ are the magnetoelectric dyadics. Substituting (1) into the source–free Maxwell curl postulates, we obtain the dyadic differential equation

$$\underline{\underline{\mathbf{L}}}(\nabla) \cdot \underline{\mathbf{F}}(\underline{r}) = -i\omega \underline{\underline{\mathbf{K}}}(\underline{r}) \cdot \underline{\mathbf{F}}(\underline{r}) \,, \tag{2}$$

[1] Whereas 3–vectors (6–vectors) are in normal (bold) face and underlined, 3×3 dyadics (6×6 dyadics) are in normal (bold) face and underlined twice. The adjoint, determinant and inverse of the dyadic $\underline{\underline{\mathbf{Q}}}$ are denoted by adj($\underline{\underline{\mathbf{Q}}}$), det $\underline{\underline{\mathbf{Q}}}$ and $\underline{\underline{\mathbf{Q}}}^{-1}$, respectively.

where

$$\underline{\underline{\mathbf{L}}}(\nabla) = \begin{bmatrix} \underline{\underline{0}} & \nabla \times \underline{\underline{I}} \\ -\nabla \times \underline{\underline{I}} & \underline{\underline{0}} \end{bmatrix}, \qquad \underline{\underline{\mathbf{K}}}(\underline{r}) = \begin{bmatrix} \underline{\underline{\epsilon}}(\underline{r}) & \underline{\underline{\xi}}(\underline{r}), \\ \underline{\underline{\zeta}}(\underline{r}) & \underline{\underline{\mu}}(\underline{r}) \end{bmatrix}, \qquad \underline{\mathbf{F}}(\underline{r}) = \begin{bmatrix} \underline{E}(\underline{r}) \\ \underline{H}(\underline{r}) \end{bmatrix}, \tag{3}$$

with $\underline{\underline{I}}$ denoting the 3×3 unit dyadic.

Equation (2) is specialized to a two–phase composite mixed at the microscopic (but not molecular) length scale, each constituent material phase taken to be bianisotropic as follows: All space is divided into disjoint parts V_a and V_b such that

$$\underline{\underline{\epsilon}}(\underline{r}) = \underline{\underline{\epsilon}}_p\,, \quad \underline{\underline{\xi}}(\underline{r}) = \underline{\underline{\xi}}_p\,, \quad \underline{\underline{\zeta}}(\underline{r}) = \underline{\underline{\zeta}}_p\,, \quad \underline{\underline{\mu}}(\underline{r}) = \underline{\underline{\mu}}_p \quad \Rightarrow \quad \underline{\underline{\mathbf{K}}}(\underline{r}) = \underline{\underline{\mathbf{K}}}_p\,, \qquad \underline{r} \in V_p\,. \tag{4}$$

We introduce the characteristic function $\theta_p(\underline{r})$, defined as

$$\theta_p(\underline{r}) = 1\,, \qquad \underline{r} \in V_p\,; \qquad\qquad \theta_p(\underline{r}) = 0\,, \qquad \underline{r} \notin V_p\,. \tag{5}$$

The complete statistical information about the composite is contained in $\theta_p(\underline{r})$. On average, the composite is assumed to be homogeneous.

The concept of ensemble–averaging, i.e., averaging over a large number of different samples of the two–phase composite, is central to the SPFT. With ensemble–averages denoted by $\langle\ \rangle$, the nth moment of $\theta_p(\underline{r})$ is the expectation value $\langle \theta_p(\underline{r}_1)\ldots\theta_p\underline{r}_n)\rangle$, which represents the probability for $\underline{r}_1, \ldots, \underline{r}_n$ being inside V_p. The first moment for the phase p is its volume fraction $f_p = \langle\theta_p(\underline{r})\rangle$. Only f_p, $(p = a, b)$ appear in the Maxwell Garnett and the Bruggeman formalisms, which thus contain minimal statistical information about the composite. A more detailed description is provided by the second moment $\langle\theta_a(\underline{r})\theta_a(\underline{r}')\rangle$ of $\theta_a(\underline{r})$, or, equivalently, by the second *cumulant* or *covariance*

$$\tau(\underline{R}) = \langle\theta_a(\underline{r})\theta_a(\underline{r}')\rangle - \langle\theta_a(\underline{r})\rangle\langle\theta_a(\underline{r}')\rangle = \langle\theta_b(\underline{r})\theta_b(\underline{r}')\rangle - \langle\theta_b(\underline{r})\rangle\langle\theta_b(\underline{r}')\rangle\,, \tag{6}$$

where $\underline{R} = \underline{r} - \underline{r}'$. If the composite is disordered, it is usually possible to define a correlation length L such that $\tau(\underline{R})$ is negligible for $|\,\underline{R}\,| \gg L$; i.e., on scales larger than L, the composite may be considered homogeneous.

The formulation of SPFT requires the introduction of a bianisotropic comparison medium (BCM), which allows an approximate treatment of electromagnetic fields in $V_a \cup V_b$. This is a homogeneous medium, characterized by the constitutive dyadic $\underline{\underline{\mathbf{K}}}_{BCM}$, which serves as the preliminary ansatz for the SPFT and may be chosen as the result of implementing the Bruggeman formalism [5]. The corresponding dyadic Green function $\underline{\underline{\mathbf{G}}}_{BCM}(\underline{r} - \underline{r}')$ satisfies the differential equation

$$\left[\underline{\underline{\mathbf{L}}}(\nabla) + i\omega\underline{\underline{\mathbf{K}}}_{BCM}\right] \bullet \underline{\underline{\mathbf{G}}}_{BCM}(\underline{r} - \underline{r}') = \underline{\underline{\mathbf{I}}}\,\delta(\underline{r} - \underline{r}')\,, \tag{7}$$

where $\underline{\underline{\mathbf{I}}}$ is the unit 6×6 dyadic and $\delta(\underline{r} - \underline{r}')$ is the Dirac delta function. The singular behaviour of $\underline{\underline{\mathbf{G}}}_{BCM}(\underline{r} - \underline{r}')$ in the limit $\underline{r} \to \underline{r}'$ can be accommodated through

$$\underline{\underline{\mathbf{G}}}_{BCM}(\underline{R}) = \mathcal{P}\underline{\underline{\mathbf{G}}}_{BCM}(\underline{R}) + \underline{\underline{\mathbf{D}}}\,\delta(\underline{R}) \tag{8}$$

where $\mathcal{P}$ is the principal value operation excluding a certain infinitesimal region centred on $\underline{R} = \underline{0}$ and the corresponding depolarization dyadic $\underline{\underline{\mathbf{D}}}$ of the specified region in the BCM [6] is fixed at a later stage in the analysis.

In the SPFT, $\underline{\underline{\mathbf{K}}}_{BCM}$ is refined in a perturbative manner in order to estimate the constitutive dyadic $\underline{\underline{\mathbf{K}}}_{Dy}(\underline{R})$ of the nonlocal effective medium arising from the homogenization of the material phases a and b. However, when the principal electromagnetic wavelengths are much larger than the correlation length L, a *macroscopic* description of the composite as a homogeneous local continuum is possible. In this long–wavelength regime, $\underline{\underline{\mathbf{K}}}_{Dy}(\underline{R}) \equiv \underline{\underline{\mathbf{K}}}_{Dy0}$, where

$$\underline{\underline{\mathbf{K}}}_{Dy0} = \underline{\underline{\mathbf{K}}}_{BCM} - \frac{1}{i\omega}\left(\underline{\underline{\mathbf{I}}} + \underline{\underline{\tilde{\mathbf{\Sigma}}}}_0 \cdot \underline{\underline{\mathbf{D}}}\right)^{-1} \cdot \underline{\underline{\tilde{\mathbf{\Sigma}}}}_0\,; \qquad \underline{\underline{\tilde{\mathbf{\Sigma}}}}_0 = \int \underline{\underline{\mathbf{\Sigma}}}(\underline{R})\, d^3\underline{R}\,. \tag{9}$$

The *mass operator* $\underline{\underline{\mathbf{\Sigma}}}(\underline{R})$ consists of an infinite series of terms involving $\mathcal{P}\underline{\underline{\mathbf{G}}}_{BCM}(\underline{R})$. The lowest–order non–trivial result emerges from the *bilocal approximation*; thus,

$$\underline{\underline{\tilde{\mathbf{\Sigma}}}}_0 = \left(\underline{\underline{\boldsymbol{\chi}}}_a - \underline{\underline{\boldsymbol{\chi}}}_b\right) \cdot \left[\mathcal{P}\int \tau(\underline{R})\, \underline{\underline{\mathbf{G}}}_{BCM}(\underline{R}) d^3\underline{R}\right] \cdot \left(\underline{\underline{\boldsymbol{\chi}}}_a - \underline{\underline{\boldsymbol{\chi}}}_b\right), \tag{10}$$

where

$$\underline{\underline{\boldsymbol{\chi}}}_p = -i\omega\left[\underline{\underline{\mathbf{K}}}_p - \underline{\underline{\mathbf{K}}}_{BCM}\right] \cdot \left[\underline{\underline{\mathbf{I}}} + i\omega \underline{\underline{\mathbf{D}}} \cdot \left(\underline{\underline{\mathbf{K}}}_p - \underline{\underline{\mathbf{K}}}_{BCM}\right)\right]^{-1}, \qquad (p = a, b). \tag{11}$$

An explicit expression for $\underline{\underline{\mathbf{G}}}_{BCM}(\underline{R})$ cannot be written down, but (7) yields its Fourier transform as

$$\underline{\underline{\tilde{\mathbf{G}}}}_{BCM}(\underline{q}) = \frac{1}{i\omega}\frac{\mathrm{adj}\left(\underline{\underline{\tilde{\mathbf{A}}}}_{BCM}(\underline{q})\right)}{\det \underline{\underline{\tilde{\mathbf{A}}}}_{BCM}(\underline{q})}\,; \qquad \underline{\underline{\tilde{\mathbf{A}}}}_{BCM}(\underline{q}) = \begin{bmatrix} \underline{\underline{0}} & (\underline{q}/\omega) \times \underline{\underline{\mathbf{I}}} \\ -(\underline{q}/\omega) \times \underline{\underline{\mathbf{I}}} & \underline{\underline{0}} \end{bmatrix} + \underline{\underline{\mathbf{K}}}_{BCM}\,, \tag{12}$$

where $\underline{q}$ is the spatial frequency vector. Significantly, $\underline{\underline{\tilde{\mathbf{G}}}}_{BCM}(\underline{q})$ may be partitioned as [6]

$$\underline{\underline{\tilde{\mathbf{G}}}}_{BCM}(\underline{q}) = \underline{\underline{\tilde{\mathbf{G}}}}^{0}_{BCM}(\underline{q}) + \underline{\underline{\tilde{\mathbf{G}}}}^{\infty}_{BCM}(\hat{\underline{q}})\,, \qquad \underline{\underline{\tilde{\mathbf{G}}}}^{\infty}_{BCM}(\hat{\underline{q}}) = \lim_{q\to\infty} \underline{\underline{\tilde{\mathbf{G}}}}_{BCM}(\underline{q}). \tag{13}$$

Let V^e_η be an ellipsoidal region, centred at the origin of our coordinate system, of size determined by the linear measure η. We imagine that both constituent phases are distributed as conformal ellipsoids of surfaces parameterized by $\underline{R}_e(\theta,\phi) = \eta\, \underline{\underline{U}} \cdot \hat{\underline{R}}(\theta,\phi)$, where $\hat{\underline{R}}(\theta,\phi)$ is the radial unit vector depending on the spherical polar coordinates θ and ϕ, and $\underline{\underline{U}}$ is a real–valued dyadic of full rank. We determine $\underline{\underline{\mathbf{D}}}$ as the depolarization dyadic associated with the exclusion region of shape $\underline{\underline{U}}$ [6] and choose the covariance $\tau(\underline{R})$ to reflect the ellipsoidal topology relating to $\underline{\underline{\mathbf{D}}}$; accordingly,

$$\tau(\underline{R}) = f_a f_b\,, \qquad \underline{R} \in V^e_L\,; \qquad\qquad \tau(\underline{R}) = 0\,, \qquad \underline{R} \notin V^e_L\,. \tag{14}$$

Thus, the principal value integral in (10) becomes

$$\begin{aligned} &\mathcal{P}\int \tau(\underline{R})\, \underline{\underline{\mathbf{G}}}_{BCM}(\underline{R})\, d^3\underline{R} = \\ &\frac{f_a f_b}{2\pi^2}\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}\int_{v=0}^{\infty} \underline{\underline{\tilde{\mathbf{G}}}}^{0}_{BCM}(\underline{\underline{U}}^{-1} \cdot \underline{v})\left(\frac{\sin vL}{v} - L\cos vL\right)\sin\theta\, dv\, d\theta\, d\phi \end{aligned} \tag{15}$$

where $\underline{v}$ is a dummy vector variable.

3. Implementation for Biaxial Bianisotropic Mediums

In order to illustrate the implementation of the long–wavelength approximation in the bilocal SPFT framework, we consider a two–phase composite for which both constituent phases belong to the general class of reciprocal biaxial bianisotropic mediums. The constitutive dyadics of the constituent phases are taken to have the diagonal forms

$$\underline{\underline{\epsilon}}_p = \mathrm{diag}(\epsilon_x^p, \epsilon_y^p, \epsilon_z^p), \quad \underline{\underline{\xi}}_p = \mathrm{diag}(\xi_x^p, \xi_y^p, \xi_z^p) = -\underline{\underline{\zeta}}_p, \quad \underline{\underline{\mu}}_p = \mathrm{diag}(\mu_x^p, \mu_y^p, \mu_z^p), \quad (p = a, b)\,, \tag{16}$$

where all diagonal entries are complex–valued. For simplicity, we choose a spherical particulate topology for the constituent phases, i.e., $\underline{\underline{U}} = \underline{\underline{I}}$. The integration with respect to v in (15) may be performed by means of residue calculus, exploiting symmetries in the integrand along the way: Introducing

$$\underline{\underline{\mathbf{N}}}(\underline{v}) = \frac{\mathrm{adj}\left(\underline{\underline{\tilde{\mathbf{A}}}}_{BCM}(\underline{v})\right) \; - \; \det\left(\underline{\underline{\tilde{\mathbf{A}}}}_{BCM}(\underline{v})\right) \underline{\underline{\tilde{\mathbf{G}}}}^{\infty}_{BCM}(\underline{\hat{v}})}{(\underline{\hat{v}} \bullet \underline{\underline{\epsilon}}_{BCM} \bullet \underline{\hat{v}})(\underline{\hat{v}} \bullet \underline{\underline{\mu}}_{BCM} \bullet \underline{\hat{v}}) + (\underline{\hat{v}} \bullet \underline{\underline{\xi}}_{BCM} \bullet \underline{\hat{v}})(\underline{\hat{v}} \bullet \underline{\underline{\xi}}_{BCM} \bullet \underline{\hat{v}})}\,, \tag{17}$$

we find that

$$\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}\int_{v=0}^{\infty} \underline{\underline{\tilde{\mathbf{G}}}}^{0}_{BCM}(\underline{v}) \left(\frac{\sin vL}{v} - L\cos vL\right) \sin\theta \, dv\, d\theta\, d\phi \; = \frac{\pi\omega^3}{4i}\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} \left\{ \frac{1}{\kappa_+ - \kappa_-} \right.$$
$$\left. \times \left[\frac{\mathrm{e}^{iLv}}{v^2}\,(1 - iLv)\left(\underline{\underline{\mathbf{N}}}(\underline{v}) + \underline{\underline{\mathbf{N}}}(-\underline{v})\right)\right]_{v=\sqrt{\kappa_-}}^{v=\sqrt{\kappa_+}} + \frac{2\,\underline{\underline{\mathbf{N}}}(\underline{0})}{\kappa_+\,\kappa_-} \right\} \sin\theta\, d\theta\, d\phi\,, \tag{18}$$

where $\kappa_\pm$ are the v^2 roots of $\det \underline{\underline{\tilde{\mathbf{A}}}}_{BCM}(\underline{v})$ and are assumed to be distinct.

4. Concluding Remarks

The constitutive dyadic $\underline{\underline{\mathbf{K}}}_{Dy0}$ is fully specified through (9), (10), (15), (17) and (18). The surface integral representation (18) requires numerical evaluation, in general; a selection of results is presented in [5]. These calculations reveal a biaxial bianisotropic composite structure which includes scattering losses, and is therefore attenuative even when the constituent material phases are nondissipative.

Acknowledgements
The work of TGM is supported by the *Carnegie Trust for the Universities of Scotland*. WSW is the holder of a *RSE/SOEID Research Support Fellowship* of the *Royal Society of Edinburgh*.

References

[1] A. Lakhtakia, "On direct and indirect scattering approaches for the homogenization of particulate composites", *Microw. Opt. Technol. Lett.* **25**, 53–56, 2000.

[2] L. Tsang and J. A. Kong, "Scattering of electromagnetic waves from random media with strong permittivity fluctuations," *Radio Sci.* **16**, 303–320, 1981.

[3] N. P. Zhuck, "Strong–fluctuation theory for a mean electromagnetic field in a statistically homogeneous random medium with arbitrary anisotropy of electrical and statistical properties," *Phys. Rev. B* **50**, 15636–15645, 1994.

[4] B. Michel and A. Lakhtakia, "Strong–property–fluctuation theory for homogenizing chiral particulate composites," *Phys. Rev. E* **51**, 5701–5707, 1995.

[5] T. G. Mackay, A. Lakhtakia and W.S. Weiglhofer, "Strong–property–fluctuation theory for homogenization of bianisotropic composites. Part I: Formulation," *Department of Mathematics, University of Glasgow*, preprint 2000/17, June 2000.

[6] B. Michel and W. S. Weiglhofer, "Pointwise singularity of dyadic Green function in a general bianisotropic medium," *Arch. Elektron. Übertrag.* **51**, 219–223, 1997; erratum: **52**, 31, 1998.