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Polarization approximations for macroscopic conductivity of isotropic multicomponent materials

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ABSTRACT

Hashin–Shtrikman-type polarization trial fields, constructed earlier by us to derive bounds on the effective conductivity of isotropic multicomponent materials, are used to derive polarization approximations for the macroscopic transport property of the d-dimensional composites ($d = 2$ or 3). The approximation contains a free parameter, which should be determined from a reference model at certain volume proportions of the component materials theoretically, numerically, or experimentally. Once the appropriate reference parameter had been chosen, the approximation would obey Hashin–Shtrikman bounds over all the ranges of volume proportions of the component materials. The approximation is expected to do best near the component-volume-proportion reference point. Numerous examples are given to illustrate the usefulness of the approach.

1. Introduction

Transport properties of many real world inhomogeneous continuum media, which include thermal and electrical conductivities (or resistivities), dielectric and magnetic permeabilities, and diffusion coefficients, are described by second rank tensors relating solenoidal vector (flux) and irrotational vector (field intensity). Technical heterogeneous materials often have complicated and irregular microgeometries, and one often has only limited definite information about the composites, such as the properties and volume proportions of the component materials. Thus, in most cases prediction of exact values of the macroscopic properties of the composites is almost impossible. A mathematically-rigorous approach to the problem is to construct upper and lower bounds on the possible values of the effective properties using various variational formulations (Elsayed, 1974; Hashin & Shtrikman, 1962; Le & Pham, 1991; Miller, 1969; Milton, 2001; Pham, 1996; 2011; Pham et al., 2013b; Phan-Thien & Milton, 1982; Torquato, 2002; Willis, 1977; 1981). When the components' properties differ largely the bounds fall far apart and do not have much practical value. Improvements of the bounds require multi-point correlation information about the microgeometries of the composites, which is difficult and costly to collect and to incorporate into the bounds. Alternatively, effective medium approximation (EMA) schemes have been developed for practical rough estimates of composites' macroscopic properties (Buryachenko, 2007; Christensen, 1979; Kanaun & Levin, 2008; Landauer, 1978; Markov et al., 2012; Mogilevskaya et al., 2012; Mori & Tanaka, 1973; Mura, 1987; Norris, 1989; Norris et al., 1985; Pham, 2008; Pham & Torquato, 2003; Phan-Thien & Pham, 2000; Sevostianov & Kachanov, 2012; Torquato, 2002; Willis, 1977; Zou et al., 2011). Most of effective medium approximations are based on dilute solutions for the inhomogeneities (mostly of idealistic spherical and ellipsoidal forms) suspended

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in an infinite matrix, and they converge at those dilute limits. However at the large volume proportions of included phases, they diverge and the simple EMAs fail to account for the effects of complex interactions between the inhomogeneities, in addition the practical inhomogeneities often do not have simple idealistic forms. Attempts to include complicated multi-particle interactions into EMAs make the approximations cumbersome, too specific, and not attractive for practical applications. With developments of high-speed high-capacity computers and digitized imaging techniques, powerful computational methods have been implemented to solve directly particular effective medium problems, from periodic to random ones (Gibson & Ashby, 1997; Flegler et al., 1993; Fredrich et al., 1995; Howle et al., 1993; Kinney & Nichols, 1992; Stroscio & Kaiser, 1993); (Bonnet, 2007; Lee, Gillman, & Matou, 2011; Michel et al., 1999; Nguyen et al., 2013; Sukumar et al., 2001; Torquato, 2002; Tran et al., 2011). For large representative volume element of a practical inhomogeneous material with complicated microgeometry, both sampling digitized images of the composite's topology and solving the respective large scale problem are costly, for just a fixed particular configuration. Lastly, empirical formulae for the conductivity of specific real-world heterogeneous media, with just a few free parameters to be determined from the respective experiments or numerical data, also are used widely and attract attentions of the practitioners in the field (Archie, 1942; Ashby et al., 2000; Lobb & Forester, 1987; Mendelson & Cohen, 1982; Mendes et al., 2014; Pham, 2000; Progelhof & Throne, 1975; Sen et al., 1981; Tobochnik et al., 1987; Zimmerman, 1989).

In this work, we propose a polarization approximation, which inherits elements of all the main approaches introduced above. In Section 2, polarization trial fields constructed earlier by us to bound the effective conductivity shall be used to derive the respective polarization approximation, which depends on a free reference parameter. This free parameter shall be determined from reference models theoretically, numerically, or experimentally in subsequent sections, which are completed by the conclusion.

2. Polarization approximation

Let us consider a representative volume element (RVE) V in d-dimensional Euclidean space ($d = 2, 3$) of an isotropic multicomponent material that consists of n components occupying regions $V_\alpha \subset V$ of volumes v_α and having conductivities c_α ($\alpha = 1, \ldots, n$; the volume of V is assumed to be the unity). The effective conductivity c^{eff} of the composite may be defined via the minimum energy principle

$$c^{eff}\mathbf{E}^0 \cdot \mathbf{E}^0 = \inf_{\langle \mathbf{E}\rangle = \mathbf{E}^0} \int_V c\mathbf{E} \cdot \mathbf{E} d\mathbf{x}, \quad (1)$$

where $\mathbf{E}$ is a gradient (intensity) field, $\mathbf{E}^0$ is a constant vector field, $\langle\cdot\rangle$ means the volume average on V, $c(\mathbf{x}) = c_\alpha$ if $\mathbf{x} \in V_\alpha$; or via the minimum complementary energy principle

$$(c^{eff})^{-1}\mathbf{J}^0 \cdot \mathbf{J}^0 = \inf_{\langle \mathbf{J}\rangle = \mathbf{J}^0} \int_V c^{-1}\mathbf{J} \cdot \mathbf{J} d\mathbf{x}, \quad (2)$$

where $\mathbf{J}$ is an equilibrated (flux) field, $\mathbf{J}^0$ is a constant vector field. With the solution fields of (1) and (2), one has the constitutive relation $\mathbf{J} = -c\mathbf{E}$.

To find a best possible upper bound on c^{eff}, instead of optimizing directly the energy expression of the difficult problem (1), we (Le & Pham, 1991; Pham, 1996) have optimized a "principal part" of it and came to Hashin–Shtrikman-type polarization trial field

$$E_i = E_i^0 - \sum_{\alpha=1}^{n} p_j^\alpha \varphi^\alpha_{,ij}, \quad i = 1, \ldots, d, \quad (3)$$

where Latin indices after comma designate differentiation with respective Cartesian coordinates; throughout this paper, the conventional summation on the repeating Latin indices from 1 to d (but not on the repeating Greek indices indicating the components) is assumed;

$$p_j^\alpha = \left[1 - \left(\sum_{\beta=1}^{n} v_\beta \frac{c_\alpha + (d-1)c_0}{c_\beta + (d-1)c_0}\right)^{-1}\right] dE_j^0, \quad (4)$$

φ^α are the harmonic potentials

$$\varphi^\alpha(\mathbf{x}) = \int_{V_\alpha} G(\mathbf{x}-\mathbf{y})d\mathbf{y}\,; \quad \nabla^2\varphi^\alpha(\mathbf{x}) = \delta_{\alpha\beta}, \quad \mathbf{x} \in V_\beta;$$

$$G(\mathbf{x}) = \begin{cases} \dfrac{1}{2\pi}\ln|\mathbf{x}|, & d = 2 \\ -\dfrac{1}{4\pi|\mathbf{x}|}, & d = 3 \end{cases}, \quad (5)$$

$\delta_{\alpha\beta}$ is Kröneker symbol. Because of macroscopic isotropy one has

$$\left\langle \varphi^\alpha_{,ij} \right\rangle_\beta = \frac{1}{d}\delta_{\alpha\beta}\delta_{ij}, \quad (6)$$