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JUSTIFICATION OF AN EFFECTIVE FIELD METHOD IN ELASTO-STATICS OF HETEROGENEOUS SOLIDS

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ABSTRACT

A heuristic scheme for predicting the overall properties of composite media has been proposed, explored and widely used in the last 25 years by Kanaun and Levin. The numerous results and technical details are collected in the impressive volume Kanaun and Levin (1993 Petrozavodsk: Izdatel'stvo Petrozavodskogo Universiteta [in Russian]). The method is based on a certain old, natural and appealing physical reasoning, which well explains its name *effective field method* (EFM). The predictions of the methods agree very well with many experimental data. However, no attempt has been made to justify the method, putting it into the frame of a more rigorous theory of heterogeneous media. The present study represents such an attempt. The main conclusion is that the EFM approach, at least in elasto-statics when the effective moduli of the composite are looked for, is in essence a variational procedure of Hashin-Shtrikman' type. Hence Kanaun–Levin's results provide, for the microstructures treated by the authors, rigorous variational prescriptions. The latter represent bounds on the effective moduli of the composites, if the matrix is weaker or stiffer than the inclusions. Moreover, it is shown that in the special, though quite general case of a matrix containing several kinds of ellipsoidal inclusions, distributed with "ellipsoidal" symmetry, an obvious generalization of the EFM method yields results that coincide with the variational estimates, recently obtained by Ponte Castañeda and Willis (1995 *J. Mech. Phys. Solids* **43,** 1919–1951).

Key words: heterogeneous solids, composite media, effective properties, variational estimates

1. INTRODUCTION

Consider an elastic medium (matrix) in which $N-1$ families of particles are distributed nonoverlappingly. The rth family is a set of identical and identically oriented ellipsoids, specified by a reference domain $\Omega_{\mathrm{i}}^{(r)}$, centered at the random points $\mathbf{x}_{\alpha}^{(r)}$ $(r=2,\ldots,N)$. We assume, as usual, that the medium is statistically homogeneous. Moreover, after Willis (1977, 1978), the hypothesis of ellipsoidal symmetry is adopted. This means that the binary distribution function $p^{(rs)}(\mathbf{x},\mathbf{x}')$ that gives the probability of finding a center of rth type ellipsoid at $\mathbf{x}$ and a center of sth type one at $\mathbf{x}'$ has a special structure, namely,

$$p^{(rs)}(\mathbf{x},\mathbf{x}')=p^{(rs)}(\mathbf{x}-\mathbf{x}')=p^{(rs)}\left(\left|Z_{\mathrm{d}}^{(rs)}(\mathbf{x}-\mathbf{x}')\right|\right) \tag{1.1}$$

$(r,s=2,\ldots,N)$. Here $Z_{\mathrm{d}}^{(rs)}$ is a second-rank tensor which defines the ellipsoid

$$\Omega_{\mathrm{d}}^{(rs)}=\left\{\mathbf{x}:\left|Z_{\mathrm{d}}^{(rs)}\mathbf{x}\right|^2<1\right\}. \tag{1.2}$$

The ellipsoidal symmetry thus introduced is a convenient generalization of the notion of statistical isotropy and covers a number of interesting and important particular microstructures. Appropriate examples can be found in Ponte Castañeda and Willis (1995).

The composite occupies the region $\Omega\subset\mathcal{R}^3$, large compared to the size of the single inhomogeneities; without loss of generality we can assume that Ω is a cube of unit volume. It is then convenient to imagine that the whole $\mathcal{R}^3$ is filled with identical copies of the typical cube Ω. In this way the ensemble averaging over the set of realizations of the heterogeneous cube Ω can be replaced by the volume averaging over Ω for a specific realization. The latter averaging will be denoted by overbar.

The subject of the present work is the macroscopic elastic behaviour of the above composite medium. More precisely, we shall discuss, on the example of this specific microstructure, a heuristic scheme for evaluating the effective properties of composites that first appeared about 25 years ago in the papers of Kanaun (1975) and Levin (1976); a more "mature" exposition was given a bit later in Kanaun (1982, 1983). The scheme is based on the idea of a certain effective field acting on each particle, as a consequence of the presence of the rest of them; that is why its name *effective field method* (EFM) is entirely justified. The magnitude of the effective field is specified by means of a naturally looking "self-balance" condition. Since 1975 the scheme has been applied by Kanaun and Levin to various specific composite microstructures and considerable technical difficulties have been overcome to get explicit predictions in each particular case. The latter turned out to agree very well with many experimental data. Moreover, the obtained predictions often coincided with those, found by means of different procedures as well, or with the appropriate rigorous bounds of Hashin-Shtrikman's type. For a detailed exposition the reader is referred to the book Kanaun and Levin (1993). [The survey Kanaun and Levin (1994) is to a great extent an English summary of this book, containing in concise form all the basic ideas and the main results of the authors, both in static and dynamic cases.]

It is somewhat strange that despite the numerous publications and the reasonable and interesting results, the effective field method in Kanaun-Levin's form caused very little reaction among the scientific community, interested in effective behaviour of composites. A certain explanation may lie in the fact that most of the papers were published in Russian journals—though among those that had at that time an immediate English translation—and the Kanaun-Levin's book is also in Russian. Another reason may be sought in the terse exposition of the authors, containing many technical details. As a small historical curiosity, let us point out in passing that the paper of Mori and Tanaka (1973), published in a material sciences journal almost at the same time as the first Kanaun's paper, caused an overwhelming interest among the same community. Moreover, the original Mori-Tanaka's paper, written in an extremely concise and formal manner, did not address directly the effective properties of composites. It also turned out that the Mori-Tanaka's method, as understood today thanks to Benveniste (1987), can be treated in a sense as a particular case of the Kanaun-Levin scheme (see the end of Section 5 below).

To the best of the author's knowledge, no attempt has been made to justify the Kanaun-Levin method, putting it into the frame of a more rigorous theory of heterogeneous media. The present study represents such an attempt. The main conclusion is that the EFM approach, at least in elasto-statics when the effective moduli of the composite are looked for, is in essence a variational procedure of Hashin-Shtrikman' type. Hence Kanaun-Levin's results provide, for the microstructures treated by the authors, rigorous variational prescriptions which are bounds on the effective moduli of the composites, if the matrix is weaker or stiffer than the inclusions. Moreover, it is shown that in the special, though quite general case of a matrix containing several kinds of ellipsoidal inclusions, distributed with "ellipsoidal" symmetry, an obvious generalization of the EFM method yields results that coincide with the variational estimates, recently obtained and discussed in detail by Ponte Castañeda and Willis (1995).

The outline of the study is as follows. In Section 2 we recall the basic and well-known integral equations that govern the strain and stress fields in the composite. Section 3 is devoted to two approximate schemes for evaluating the effective properties. The first one, called a "step-constant approximation," can be traced in the paper of Willis (1982). The second one is a somewhat simplified version of the original Kanaun-Levin scheme, in which the two central and most important authors' ideas are preserved. The one is the auxiliary notion of a certain effective field acting on each single inclusion. The other is the specification of this field by means of a natural "self-balance" condition. In both approximations the "quasicrystalline" assumption of Lax (1952) plays a key role. Moreover, they both yield identical results for the strains (or, which is the same, for the polarizations within the inclusions) and hence predict the same values of the effective elastic moduli of the composite. In Section 4 the integral equation for the strain field is replaced by a variational principle, and this is exactly the Hashin-Shtrikman's one, as pointed out by Willis (1981, 1982). Then optimizing the appropriate functional using constant and adjustable polarizations within each kind of inclusions yields the estimates for the effective elastic tensor, recently obtained by Ponte Castañeda and Willis (1995). The system for the optimal polarizations of these authors turns out to coincide with the prescriptions of the Kanaun-Levin's scheme, developed in Section 3. Hence we can state that, using the microstructure under study for illustration of the reasoning, that the latter is but a variational procedure of Hashin-Shtrikman's type yielding, in this special case, the prescriptions of Ponte Castañeda and Willis (1995). The analysis allows us to conclude the study with several simple observations (Section 5). They concern, e.g. the condition needed for the well-known approximation of Mori-Tanaka (1973) to supply a rigorous bound on the effective elastic moduli of a dispersion, containing aligned ellipsoidal inclusions.

2. THE INTEGRAL EQUATIONS

The elastic tensor of the material under consideration has the form

$$\mathbf{L}(\mathbf{x}) = \mathbf{L}^{(1)} + \delta\mathbf{L}(\mathbf{x}), \quad \delta\mathbf{L}(\mathbf{x}) = \sum_{r=2}^{N} \chi^{(r)}(\mathbf{x})\delta\mathbf{L}^{(r)}, \qquad \delta\mathbf{L}^{(r)} = \mathbf{L}^{(r)} - \mathbf{L}^{(1)}, \tag{2.1}$$

where $\mathbf{L}^{(1)}$ and $\mathbf{L}^{(r)}$ are the elastic tensors of the matrix and of the inclusions of the rth family ($r = 2, \ldots, N$). In Eq. (2.1) $\chi^{(r)}(\mathbf{x})$ is the characteristic function of the phase 'r':

$$\chi^{(r)}(\mathbf{x}) = \sum_{\alpha=1}^{n^{(r)}} \chi_{\mathrm{i}}^{(r)}(\mathbf{x} - \mathbf{x}_\alpha^{(r)}). \tag{2.2}$$

Here $\mathbf{x}_\alpha^{(r)}$ specify the positions of the inclusions' centers of rth kind; $n^{(r)}$ is their number density. Hence the volume fraction of the rth phase is

$$c^{(r)} = n^{(r)}|\Omega_{\mathrm{i}}^{(r)}|, \quad |\Omega_{\mathrm{i}}^{(r)}| = \mathrm{vol}\,\Omega_{\mathrm{i}}^{(r)} \tag{2.3}$$

(recall that $|\Omega| = 1$).

The displacement field, $\mathbf{u}(\mathbf{x})$, in the composite is governed by the well-known equation

$$\nabla \cdot (\mathbf{L}(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{x})) = 0 \quad \text{or} \quad \nabla \cdot (\mathbf{L}^{(1)}(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{x})) + \nabla \cdot (\delta\mathbf{L}(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{x})) = 0, \tag{2.4}$$

where $\boldsymbol{\varepsilon}(\mathbf{x}) = \frac{1}{2}(\nabla\mathbf{u} + \mathbf{u}\nabla)$ is the infinitesimal strain tensor. The usual boundary condition applies

$$\mathbf{u}(\mathbf{x}) \Big|_{\partial\Omega} = \boldsymbol{\varepsilon}_0 \cdot \mathbf{x}, \tag{2.5}$$

with a fixed symmetric second-rank tensor $\boldsymbol{\varepsilon}_0$.

Eq. (2.4) can be replaced by the integral equation

$$\boldsymbol{\varepsilon} + \mathcal{G}\Big(\delta\mathbf{L}\boldsymbol{\varepsilon} - \overline{\delta\mathbf{L}\boldsymbol{\varepsilon}}\Big) = \boldsymbol{\varepsilon}_0, \tag{2.6}$$

where $\mathcal{G}$ stands for the integral operator

$$(\mathcal{G}\boldsymbol{\psi})(\mathbf{x}) = \int \boldsymbol{\Gamma}(\mathbf{x} - \mathbf{x}')\boldsymbol{\psi}(\mathbf{x}')\, \mathrm{d}\mathbf{x}', \tag{2.7}$$

and the overbar, let us recall, indicates averaging over the typical cube Ω. Here $\boldsymbol{\psi}$ is a second-rank tensor field and the integration is spread over the whole $\mathcal{R}^3$. In Eq. (2.7) the Cartesian components of the fourth-rank tensor $\boldsymbol{\Gamma}$ read

$$\Gamma_{ijkl}(\mathbf{x}) = -\frac{\partial^2 G_{ik}(\mathbf{x})}{\partial x_j \partial x_l}\Bigg|_{(ij)(kl)}, \tag{2.8}$$

with $G_{ik}(\mathbf{x})$ denoting the components of the Green tensor for an unbounded elastic solid possessing the elastic tensor $\mathbf{L}^{(1)}$ of the matrix. Of course, a more rigorous reasoning would require that the finite-body Green function $G_{ij}(x; x')$ be used in Eqs. (2.7) and (2.8). But it has been tacitly assumed from the very beginning that the size of the inclusions is negligibly small when compared to that of the typical cube Ω; that is why the integration in Eq. (2.7) is over the whole $\mathcal{R}^3$ and the Green tensor that shows up is chosen as the one for an unbounded medium, see, e.g., Willis (1977, 1981).

Note that an averaging of both sides of Eq. (2.7) yields $\overline{\boldsymbol{\varepsilon}} = \boldsymbol{\varepsilon}_0$, as it should be. [Recall that the boundary condition (2.5) uniquely determines the average strain within the volume Ω, according to a well-known result, see, e.g. Hill (1963) *et al.*]

A straightforward application of the Hooke law in Eq. (2.6) yields the familiar integral equation with respect to the stress field $\boldsymbol{\sigma}(\mathbf{x})$:

$$\boldsymbol{\sigma} + \mathcal{S}\Big(\delta\mathbf{M}\boldsymbol{\sigma} - \overline{\delta\mathbf{M}\boldsymbol{\sigma}}\Big) = \boldsymbol{\sigma}_0, \tag{2.9}$$

where

$$\delta\mathbf{M}(\mathbf{x}) = \mathbf{M}(\mathbf{x}) - \mathbf{M}^{(1)}, \quad \mathbf{M}(\mathbf{x}) = \mathbf{L}^{-1}(\mathbf{x}), \quad \mathbf{M}^{(1)} = \Big(\mathbf{L}^{(1)}\Big)^{-1}, \tag{2.10}$$

are the appropriate compliances tensors, and $\boldsymbol{\sigma}_0 = \mathbf{L}^{(1)}\boldsymbol{\varepsilon}_0$. The integral operator $\mathcal{S}$ in Eq. (2.9) has the convolution form (2.7) with the well-known kernel

$$\boldsymbol{S}(\mathbf{x}) = \delta(\mathbf{x})\mathbf{L}^{(1)} - \mathbf{L}^{(1)}\boldsymbol{\Gamma}(\mathbf{x})\mathbf{L}^{(1)}, \tag{2.11}$$

often called in the literature Green's stress tensor.

Note that the kernels $\boldsymbol{\Gamma}$ and $\boldsymbol{S}$ of the integral operators $\mathcal{G}$ and $\mathcal{S}$, respectively, should be treated as generalized functions, since their kernels have the singularity $|\mathbf{x}|^{-3}$. Their proper definition, when applied to constant field (the regularization) has been discussed by Kanaun (1977), see also Kanaun (1983). It turns out that for a prescribed *constant* strain field $\boldsymbol{\varepsilon}_0$, one has

$$\mathcal{G}\boldsymbol{\psi} = (\mathbf{L}^{(1)})^{-1}\boldsymbol{\psi}, \quad \mathcal{S}\boldsymbol{\psi} = 0, \quad \boldsymbol{\psi} = \text{const.} \tag{2.12}$$

The integral equations (2.6) and (2.9) can be recast, after Willis (1981, 1982), as

$$\delta\mathbf{L}^{-1}\boldsymbol{\tau} + \mathcal{G}\Big(\boldsymbol{\tau} - \overline{\boldsymbol{\tau}}\Big) = \boldsymbol{\varepsilon}_0, \tag{2.13a}$$

$$\delta\mathbf{M}^{-1}\boldsymbol{\mu} + \mathcal{S}\Big(\boldsymbol{\mu} - \overline{\boldsymbol{\mu}}\Big) = \boldsymbol{\sigma}_0, \tag{2.13b}$$

$$\boldsymbol{\tau} = \delta\mathbf{L}\boldsymbol{\varepsilon}, \quad \boldsymbol{\mu} = \delta\mathbf{M}\boldsymbol{\sigma}, \tag{2.14}$$

are, respectively, the stress and strain polarization fields. The invertibility of the tensors $\delta\mathbf{L}(\mathbf{x})$ and $\delta\mathbf{M}(\mathbf{x})$ has been assumed in Eqs. (2.13). It will hold, in particular, if $\delta\mathbf{L} > 0$ or $\delta\mathbf{L} < 0$, i.e. if the matrix is the weakest or the most rigid of the constituents. Both these cases will be of central importance in the sequel, since the proposed formulae for the effective properties will be then rigorous bounds on the tensor $\mathbf{L}^*$.

In the particular case, when the cube contains a single inclusion $\Omega_{\mathrm{i}}^{(r)}$ of the rth material, Eq. (2.6) implies

$$\begin{aligned} &\boldsymbol{\varepsilon} = \mathbf{A}^{(r)}\boldsymbol{\varepsilon}_0, \quad \mathbf{x} \in \Omega_{\mathrm{i}}^{(r)}, \\ &\mathbf{A}^{(r)} = \Big(\mathbf{I} + \mathbf{P}_{\mathrm{i}}^{(r)}\delta\mathbf{L}^{(r)}\Big)^{-1}, \quad \mathbf{P}_{\mathrm{i}}^{(r)} = \int_{\Omega_{\mathrm{i}}^{(r)}} \boldsymbol{\Gamma}(\mathbf{x})\,\mathrm{d}\mathbf{x}, \end{aligned} \tag{2.15}$$

since $\overline{\delta\mathbf{L}\boldsymbol{\varepsilon}} = 0$ in the case under study (the size of the single inclusion is vanishingly small as compared to the cube Ω). In Eq. (2.15) $\mathbf{I}$ is the fourth-rank unit tensor; $\mathbf{P}_{\mathrm{i}}^{(r)}$ is the familiar $\mathbf{P}$-tensor for the rth type of inclusions ($r = 2, \ldots, N$). Its explicit expression for the ellipsoids under study can be found, e.g. in Mura (1988) or in Ponte Castañeda and Willis (1995).

3. TWO APPROXIMATE SCHEMES

The definition of the polarization field $\boldsymbol{\tau}$, cf. Eq. (2.14), implies

$$\overline{\boldsymbol{\sigma}} = \mathbf{L}^*\overline{\boldsymbol{\varepsilon}} = \mathbf{L}^{(1)}\overline{\boldsymbol{\varepsilon}} + \overline{\boldsymbol{\tau}}.$$

Here $\mathbf{L}^*$ is the effective elastic tensor of the composite. In turn,

$$\overline{\boldsymbol{\tau}} = \sum_{r=2}^{N} \overline{\boldsymbol{\tau}^{(r)}} = \overline{\delta \mathbf{L} \boldsymbol{\varepsilon}} = \sum_{r=2}^{N} c^{(r)} \delta \mathbf{L}^{(r)} \langle \boldsymbol{\varepsilon} \rangle_r, \tag{3.1}$$

where $\boldsymbol{\tau}^{(r)} = \delta \mathbf{L}^{(r)} \boldsymbol{\varepsilon}$, $\mathbf{x} \in \Omega_{\mathrm{i}}^{(r)}$, and

$$\langle \cdot \rangle_r = \frac{1}{|\Omega^{(r)}|} \int_{\Omega^{(r)}} \cdot \, \mathrm{d}\mathbf{x} \tag{3.2}$$

stands for averaging over the volume $\Omega^{(r)}$, occupied by the phase 'r'. Hence

$$\overline{\boldsymbol{\sigma}} = \mathbf{L}^* \overline{\boldsymbol{\varepsilon}} = \mathbf{L}^{(1)} \overline{\boldsymbol{\varepsilon}} + \sum_{r=2}^{N} c^{(r)} \delta \mathbf{L}^{(r)} \langle \boldsymbol{\varepsilon} \rangle_r. \tag{3.3}$$

It is noted that the homogeneity assumption allows us to replace the averaging $\langle \cdot \rangle_r$ with an averaging over the appropriate representative ellipsoid $\Omega_{\mathrm{i}}^{(r)}$:

$$\langle \cdot \rangle_r = \frac{1}{|\Omega_{\mathrm{i}}^{(r)}|} \int_{\Omega_{\mathrm{i}}^{(r)}} \cdot \, \mathrm{d}\mathbf{x} \tag{3.4}$$

$(r = 2, \ldots, N)$. Therefore only the strains within $\Omega_{\mathrm{i}}^{(r)}$ $(r = 2, \ldots, N)$ are needed in order to evaluate the effective elastic tensor $\mathbf{L}^*$.

The boundary-value problem (2.4), (2.5) is linear with respect to the macroscopic field $\boldsymbol{\varepsilon}_0$. To find $\mathbf{L}^*$ it thus suffices to interconnect $\boldsymbol{\varepsilon}_0$ and the local strains $\langle \boldsymbol{\varepsilon} \rangle_r$ within the inclusions. Various approximations that exist in the literature on composite media provide various ways for such an interconnection, guided by certain plausible arguments. The most widely used are the "one-particle" approximations in which the single-ellipsoid solution (2.15) is appropriately utilized; many details with the basic references can be found in the recent author's survey (Markov, 2000).

Here we shall propose two more approximate schemes. As it will turn out they are equivalent. In the next section we shall justify them—in the sense that both will give results coinciding with the rigorous variational prescriptions that follow from the Hashin-Shtrikman variational principle.

3.1. The "step-constant approximation"

Imagine that the strains, acting within the inclusions of rth kinds, are *constant*, equaling $\boldsymbol{\varepsilon}^{(r)}$ $(r = 2, \ldots, N)$ [using Kanaun's coinage (Kanaun, 1982), we shall call this the **H1**-*hypothesis*]. That is why the scheme to be described below, can be called "step-constant approximation." As a matter of fact, it was discussed by Willis (1982), in the context of a Hashin-Shtrikman's variational procedure [see Sections 4 and 5 below].

Let us fix the point $\mathbf{x}$ within the inclusion $\Omega_{\rm i}^{(r)}$. Then under the hypothesis **H1**, the integral equation (2.6) yields the approximation

$$\boldsymbol{\varepsilon}^{(r)} + \sum_{s=2}^{N} \int \boldsymbol{\Gamma}(\mathbf{x}-\mathbf{y})\delta\mathbf{L}^{(s)}\boldsymbol{\varepsilon}^{(s)}\Big[\,\chi^{(s)}(\mathbf{y}) - c^{(s)}\,\Big]\,\mathrm{d}\mathbf{y} = \boldsymbol{\varepsilon}_0, \quad \mathbf{x}\in\Omega_{\rm i}^{(r)} \qquad (3.5)$$

$(r = 2,\ldots,N)$. Since Eq. (3.5) is to hold for *any* inclusion of rth kind, we can recast it in the form

$$\chi^{(r)}(\mathbf{x})\boldsymbol{\varepsilon}^{(r)} + \chi^{(r)}(\mathbf{x})\sum_{s=2}^{N} \int \boldsymbol{\Gamma}(\mathbf{x}-\mathbf{y})\delta\mathbf{L}^{(s)}\boldsymbol{\varepsilon}^{(s)}\Big[\,\chi^{(s)}(\mathbf{y}) - c^{(s)}\,\Big]\,\mathrm{d}\mathbf{y} = \chi^{(r)}(\mathbf{x})\boldsymbol{\varepsilon}_0, \qquad (3.6)$$

recalling that $\chi^{(r)}(\mathbf{x})$ is the characteristic function of the region, occupied by the constituent 'r', within which $\boldsymbol{\varepsilon}^{(r)}$ is assumed constant $(r = 2,\ldots,N)$.

It is noted that Eqs. (3.5) and (3.6) are clearly approximations, since the integrals in their left-hand sides produce strains that cannot be constant within the inclusions $\Omega_{\rm i}^{(r)}$.

Eq. (3.6) obviously suggests an averaging over the cube Ω in the hope to get explicit equations for the strains $\boldsymbol{\varepsilon}^{(r)}$ and also to get rid of their fluctuations within $\Omega_{\rm i}^{(r)}$, induced by the above mentioned integrals. The fields $\chi^{(s)}(\mathbf{x})$ are however random, as well as the unknowns $\boldsymbol{\varepsilon}^{(r)}$ and, in general, $\boldsymbol{\varepsilon}^{(r)}$ are *correlated* with $\chi^{(s)}(\mathbf{x})$. (In other words, $\boldsymbol{\varepsilon}^{(r)}$ are sensitive to the presence and locations of the inclusions, surrounding $\Omega_{\rm i}^{(r)}$.) Hence, simple results can only be expected, if a second basic hypothesis, to be called **H2** again after Kanaun (1982), is adopted. It states that the strains $\boldsymbol{\varepsilon}^{(r)}$ and the characteristic functions $\chi^{(s)}(\mathbf{x})$ of the phases are uncorrelated $(r, s = 2,\ldots,N)$. This assumption is just the "quasicrystalline" approximation of Lax (1952), as pointed out by Willis (1982). [The same fact was explicitly mentioned by Kanaun (1982) as well.]

Under the hypothesis **H2** an averaging of Eq. (3.6) gives

$$c^{(r)}\boldsymbol{\varepsilon}^{(r)} + \sum_{s=2}^{N} \overline{A^{(rs)}}\,\delta\mathbf{L}^{(s)}\boldsymbol{\varepsilon}^{(s)} = c^{(r)}\boldsymbol{\varepsilon}_0, \qquad (3.7)$$

where

$$A^{(rs)} = \iint \chi^{(r)}(\mathbf{x})\Big[\,\chi^{(s)}(\mathbf{x}') - c^{(s)}\,\Big]\boldsymbol{\Gamma}(\mathbf{x}-\mathbf{x}')\,\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}' \qquad (3.8)$$

is the statistical quantity, introduced, e.g., by Willis (1977) $(r, s = 2,\ldots,N)$. For the particular ("ellipsoidal") statistics under study, the average value of $A^{(rs)}$ was evaluated by Ponte Castañeda and Willis (1995). Their result reads:

$$\overline{A^{(rs)}} = c^{(r)}\Big(\delta_{rs}\mathbf{P}_{\rm i}^{(r)} - c^{(s)}\mathbf{P}_{\rm d}^{(rs)}\Big), \qquad (3.9)$$

where $\mathbf{P}_{\rm d}^{(rs)}$ is the $\mathbf{P}$-tensor (2.15), corresponding to the ellipsoid $\Omega_{\rm d}^{(rs)}$ that defines the pair distribution of the rth and sth kinds of inclusions [see Section 1 and Eq. (1.2)].

From Eqs. (3.7) and (3.9) one gets the linear system

$$\left[\mathbf{I} + \mathbf{P}_{\mathrm{i}}^{(r)} \delta \mathbf{L}^{(r)}\right] \boldsymbol{\varepsilon}^{(r)} - \sum_{s=2}^{N} c^{(s)} \mathbf{P}_{\mathrm{d}}^{(rs)} \delta \mathbf{L}^{(s)} \boldsymbol{\varepsilon}^{(s)} = \boldsymbol{\varepsilon}_0 \tag{3.10}$$

for the unknowns $\boldsymbol{\varepsilon}^{(r)}$ $(r, s = 2, \ldots, N)$. It can be explicitly solved for a prescribed microstructure (i.e. for the given tensors $\mathbf{P}_{\mathrm{i}}^{(r)}$ and $\mathbf{P}_{\mathrm{d}}^{(rs)}$ that reflect the shape of the inclusions and their mutual binary distribution, respectively). Replacing $\langle \boldsymbol{\varepsilon} \rangle_r$ in Eq. (3.3) by the so-obtained $\boldsymbol{\varepsilon}^{(r)}$ one explicitly finds in turn a certain value of the effective elastic tensor $\mathbf{L}^*$ of the medium, within the frame of the approximate scheme under consideration.

3.2. The "effective field" approximation

Utilizing the old "cavity" idea of Mossotti, let us "cut out" the rth reference inclusion $\Omega_{\mathrm{i}}^{(r)}$ from the medium, replacing it by a cavity. More precisely, in the context of particulate composites, this means first of all that the region in $\mathcal{R}^3$, occupied by $\Omega_{\mathrm{i}}^{(r)}$ is considered. If it were filled with matrix material (hence removing the inhomogeneity), a certain strain field $\boldsymbol{\varepsilon}_{\mathrm{eff}}^{(r)}$ will be acting throughout this region, as a result of the presence of the rest of the inclusions. For simplicity, we shall assume it constant, guided by the fact that the inclusions are small macroscopically and, as a first approximation, there is no need to account for the strain fluctuations in the regions $\Omega_{\mathrm{i}}^{(r)}$; moreover it is fully natural as well to imagine $\boldsymbol{\varepsilon}_{\mathrm{eff}}^{(r)}$ *different* for different kinds of inclusions $(r = 2, \ldots, N)$. Then $\boldsymbol{\varepsilon}_{\mathrm{eff}}^{(r)}$ is the familiar *effective field* that often reappeared in different disguises in theory of heterogeneous media. In dielectric context, for instance, the foregoing effective field is tantamount to the well-known local field, called Lorenz-Lorentz's in the physical literature [see, e.g. Brown (1956) or Feynman *et al.* [1964, Ch. 11.5] for a "cavity" derivation of the classical Clausius-Mossotti's formula for the dielectric permittivity.]

Now, when the inclusion $\Omega_{\mathrm{i}}^{(r)}$ is put back into its place in the medium, one can treat it as a single one, lying in the external field $\boldsymbol{\varepsilon}_{\mathrm{eff}}^{(r)}$.[1] Hence,

$$\boldsymbol{\varepsilon}^{(r)} = \langle \boldsymbol{\varepsilon} \rangle_r = \mathbf{A}^{(r)} \boldsymbol{\varepsilon}_{\mathrm{eff}}^{(r)}, \quad \mathbf{x} \in \Omega_{\mathrm{i}}^{(r)}, \tag{3.11}$$

where the "single-inclusion" tensor $\mathbf{A}^{(r)}$ is given in (2.15). In virtue of Eqs. (3.3) and (3.4) it is clear that the effective tensor $\mathbf{L}^*$ would be immediately specified, once the effective fields $\boldsymbol{\varepsilon}_{\mathrm{eff}}^{(r)}$ are expressed through the microscopical strain $\overline{\boldsymbol{\varepsilon}}$. [Of course, it is not necessary to assume the effective fields constant, but then the "single-inclusion"

[1]If the foregoing "cavity" arguments are hard to digest for a modern reader, one can simply state that each inclusion is treated as single, lying in a certain external field that differs from the microscopical one, due to the presence of other inclusions. This is just the starting point of Kanaun and Levin's approach in the theory of composite media.

tensors $\mathbf{A}^{(r)}$ would be more complicated, and an averaging over the inclusion volume would be unavoidable.]

Since $\boldsymbol{\varepsilon}_{\text{eff}}^{(r)}$ are treated as certain strain fields that act throughout the specimen, they should be "self-balanced." This means, more precisely, that they should satisfy certain conditions which stem from the integral equation (2.6) that governs the strains within the composite medium. These conditions obviously read

$$\begin{aligned} \boldsymbol{\varepsilon}_{\text{eff}}^{(r)} + \mathcal{G}\left(\delta\mathbf{L}^{(r)}\boldsymbol{\varepsilon}^{(r)}\left[\sum_{\substack{\alpha=1\\ \alpha\neq i}}^{n^{(r)}}\chi_{\text{i}}^{(r)}\left(\mathbf{x}-\mathbf{x}_{\alpha}^{(r)}\right)-c^{(r)}\right]\right) \\ + \sum_{\substack{s=2\\ s\neq r}}^{N}\mathcal{G}\left(\delta\mathbf{L}^{(s)}\boldsymbol{\varepsilon}^{(s)}\left[\sum_{\alpha=1}^{n^{(s)}}\chi_{\text{i}}^{(s)}\left(\mathbf{x}-\mathbf{x}_{\alpha}^{(s)}\right)-c^{(s)}\right]\right) = \boldsymbol{\varepsilon}_0, \quad \mathbf{x}\in\Omega_{\text{i}}^{(r)} \end{aligned} \tag{3.12}$$

$(r = 2, \ldots, N)$. In words, the strain inside the given inclusion results from the influence of the appropriate strain fields, imposed upon all inclusions, *except* for the fixed one, $\Omega_{\text{i}}^{(r)}$.

In Eq. (3.12) we have tacitly assumed that the reference inclusion $\Omega_{\text{i}}^{(r)}$ of the rth kind is just the one with the index 'i', so that

$$\Omega_{\text{i}}^{(r)} = \left\{\mathbf{x}\in\Omega \;:\; h^{(r)}\left(\mathbf{x}-\mathbf{x}_{i}^{(r)}\right)\neq 0\right\}, \tag{3.13}$$

where $h^{(r)}(\mathbf{x})$ is the characteristic function of an ellipsoid of the rth type, located at the origin $(r = 2, \ldots, N)$.

Recast Eq. (3.12) as

$$\begin{aligned} \boldsymbol{\varepsilon}_{\text{eff}}^{(r)} - \mathcal{G}\left(\delta\mathbf{L}^{(r)}\boldsymbol{\varepsilon}^{(r)}h^{(r)}\left(\mathbf{x}-\mathbf{x}_{i}^{(r)}\right)\right) \\ + \sum_{s=2}^{N}\mathcal{G}\left(\delta\mathbf{L}^{(s)}\boldsymbol{\varepsilon}^{(s)}\left[\chi^{(s)}(\mathbf{x})-c^{(s)}\right]\right) = \boldsymbol{\varepsilon}_0, \quad \mathbf{x}\in\Omega_{\text{i}}^{(r)}, \end{aligned} \tag{3.14}$$

cf. (2.2) and (3.13). But

$$\mathcal{G}\left(\delta\mathbf{L}^{(r)}\boldsymbol{\varepsilon}^{(r)}h^{(r)}\left(\mathbf{x}-\mathbf{x}_{i}^{(r)}\right)\right) = \mathbf{P}_{\text{i}}^{(r)}\delta\mathbf{L}^{(r)}\boldsymbol{\varepsilon}^{(r)}, \tag{3.15}$$

as it follows from Eqs. (2.7) and (2.15). On the other hand,

$$\boldsymbol{\varepsilon}_{\text{eff}}^{(r)} = \left(\mathbf{A}^{(r)}\right)^{-1}\boldsymbol{\varepsilon}^{(r)} = \left[\,\mathbf{I}+\mathbf{P}_{\text{i}}^{(r)}\delta\mathbf{L}^{(r)}\,\right]\boldsymbol{\varepsilon}^{(r)}, \tag{3.16}$$

see again (2.15) and also (3.11). Eqs. (3.15) and (3.16), when inserted into (3.14), yield the already known relation (3.5). Employing once more the hypothesis **H2**—statistical independence of the local fields [or, which is the same, of the strains $\boldsymbol{\varepsilon}^{(r)}$] and the location of the particles—we can identically repeat the reasoning after (3.5) and reach the *same* system (3.10) for the strains $\boldsymbol{\varepsilon}^{(r)}$ inside the inclusions. Hence the two approximate schemes, described in this section, are indeed equivalent, provided the two basic hypotheses **H1** and **H2** are adopted.

It is remarked that the same results can be obtained, if instead of the integral equation (2.6) for the strain, Eq. (2.9) for the stress field is used as a starting point. The appropriate reasoning is to be repeated almost literally, replacing effective strains with effective stresses, elastic tensors with elastic compliances, and so forth.

3.3. Discussion of the approximations

The above reasoning (Section 3.2) is a simplified version of the Kanaun-Levin's scheme, generalized in the sense that different local fields are allowed to act upon different kinds of inclusions.[2] Two of the central and most important points of the scheme have been preserved and underlined at the same time. The first is the idea of the local field, acting on each inclusion, and its independence of the exact location of the surrounding particles (the **H2**-hypothesis). The second is the "self-balance" of the local effective fields, reflected by Eq. (3.5). The original Kanaun-Levin's scheme looks at first glance more complicated: the local strains $\boldsymbol{\varepsilon}_{\text{eff}} = \boldsymbol{\varepsilon}_{\text{eff}}(\mathbf{x})$ are treated there as a certain unknown random field from the very beginning, to be specified by the same Eq. (3.5). "Quasicrystalline" type of hypotheses, the simplest of which is **H2**, are then utilized in order to split the two "interwoven" problems. The first is to find the mean values $\overline{\boldsymbol{\varepsilon}}_{\text{eff}}$ within the inclusions, the second—to find the multi-point correlations of $\boldsymbol{\varepsilon}_{\text{eff}}(\mathbf{x})$. [Once found, the latter make possible the evaluation of the similar correlations for the stress and strain fields, see Kanaun (1982, 1983) or Kanaun and Levin (1993) for details.] Our reasoning in Section 3.2 is simplified, but equivalent, to that of Kanaun and Levin, under the simplest **H2**-hypothesis, in the sense that it directly yields the needed system for the mean values of the local strains [$\boldsymbol{\varepsilon}^{(r)}$ in our notations]. There is no need to bother hence for the higher-order correlation functions, within the frame of our reasoning. And this is good, in author's view, since the usefulness of Kanaun-Levin's procedure, as far as the correlation functions are concerned, is questionable: they would be only certain approximations, with *no* information, available in the moment, about their reliability and/or connection with the real ones. At the same time the situation with the overall moduli, as predicted by Kanaun-Levin's scheme in its simplified and generalized form of Section 3.2, turns out to be drastically different. Namely, the appropriate predictions appear to coincide with some rigorous Hashin-Shtrikman's type prescriptions on the effective tensor $\mathbf{L}^*$. This important fact, central for the present study, will be demonstrated in the next section on the example of the "ellipsoidal" particulate microstructure, described in Section 1.

[2]Very recently, in a private communication, Levin informed the author that Kanaun had generalized their original reasoning, also allowing different effective fields to act upon different kinds of particles in multi-phase media.

4. THE HASHIN-SHTRIKMAN PRINCIPLE AND THE JUSTIFICATION OF THE SCHEMES

As is known the operator $(\delta\mathbf{L})^{-1}+\mathcal{G}$ is positive- or negative-definite together with $\delta\mathbf{L}$ [Willis (1977, 1981)]. Since both $(\delta\mathbf{L})^{-1}$ and $\mathcal{G}$ are symmetric operators in the space of second-rank tensors, Eq. (2.13a) is equivalent to the variational principle

$$\begin{aligned} U[\boldsymbol{\tau}(\cdot)] &= \tfrac{1}{2}\overline{\boldsymbol{\tau}(\delta\mathbf{L})^{-1}\boldsymbol{\tau}} + \tfrac{1}{2}\overline{\tau\mathcal{G}\Big(\boldsymbol{\tau}-\overline{\tau}\Big)} - \boldsymbol{\varepsilon}_0\overline{\boldsymbol{\tau}} \to \text{extr}, \\ U_{\text{extr}} &= -\tfrac{1}{2}\boldsymbol{\varepsilon}_0(\mathbf{L}^* - \mathbf{L}^{(1)})\boldsymbol{\varepsilon}_0. \end{aligned} \tag{4.1}$$

Moreover, the extremum is a minimum if $\delta\mathbf{L} \geq 0$ and a maximum if $\delta\mathbf{L} \leq 0$. As pointed out by Willis (1981, 1982), the statement (4.1) coincides with the Hashin-Shtrikman variational principle [see Hashin and Shtrikman (1962, 1963)].

After Ponte Castañeda and Willis (1995), one can plug into the functional U in (4.1) the step-constant trial polarization fields

$$\boldsymbol{\tau}(\mathbf{x}) = \sum_{s=2}^{N} \boldsymbol{\tau}^{(s)}\chi^{(s)}(\mathbf{x}), \tag{4.2}$$

and optimize with respect to the constant tensors $\boldsymbol{\tau}^{(s)}$. The technical details are given in the same paper [cf., e.g., Eq. (2.17)] and the final result [Eq. (3.19)] of these authors for the "best" $\boldsymbol{\tau}^{(s)}$ reads

$$\left[\Big(\mathbf{L}^{(r)} - \mathbf{L}^{(1)}\Big)^{-1} + \mathbf{P}_{\text{i}}^{(r)}\right]\boldsymbol{\tau}^{(r)} - \sum_{s=2}^{N} c^{(s)}\mathbf{P}_{\text{d}}^{(rs)}\boldsymbol{\tau}^{(s)} = \overline{\boldsymbol{\varepsilon}} \tag{4.3}$$

$(r, s = 2, \ldots, N)$. But $\overline{\boldsymbol{\varepsilon}} = \boldsymbol{\varepsilon}_0$, and a simple comparison shows that the basic Eq. (4.3) of Ponte Castañeda and Willis that specifies the optimal polarizations $\boldsymbol{\tau}^{(s)}$ *coincides* with our Eq. (3.10) for the strain fields $\boldsymbol{\varepsilon}^{(s)}$ within the constituents, found within the frame of the approximations, discussed in Sections 3.1 and 3.2. [Recall that $\boldsymbol{\tau}^{(r)} = \delta\mathbf{L}^{(r)}\boldsymbol{\varepsilon}^{(r)}$, where $\boldsymbol{\varepsilon}^{(r)}$ is the (constant) strain within the rth constituent, see (2.14).] One can thus conclude that both approximate schemes—the step-constant and Kanaun-Levin's one—provide, on the example of the composite microstructure under study, the rigorous prescriptions of Hashin-Shtrikman's type, derived by Ponte Castañeda and Willis (1995).

The coincidence of (3.10) with the basic equation (4.3) of Ponte Castañeda and Willis (1995), specifying the optimal polarizations, means that the latter has an appealing interpretation. Namely, consider the strain fields within the composite, generated by constant strains $\boldsymbol{\varepsilon}^{(r)}$ imposed upon the inclusions $(r = 2, \ldots, N)$. Then

Eq. (4.3) simply means that these fields should be "self-balanced:" the mean strain that appears within the region, occupied by each inclusion (the Mossotti's "cavity"), should equal the external (macroscopic) field plus the mean strains, induced by the deformations $\boldsymbol{\varepsilon}^{(r)}$ of the rest of the inclusions.

5. CONCLUDING REMARKS

Several remarks are made to conclude the present study.

1. Since the integral equation (2.6) is equivalent to the variational principle (4.1), it is natural that extremizing the appropriate functional by means of step-constant trial fields is equivalent to an approximate solution of Eq. (2.9) using similar step-constant fields. We have explicitly included here the "step-constant" approximation of Section 3.1 only in order to clarify a bit the Kanaun-Levin's effective field method, as well as to underline once more the key role of the **H2**-hypothesis or, which is the same, of the Lax "quasicrystalline" assumption, and its "variational" background.

2. The starting point in Kanaun-Levin's reasoning is the integral equation (2.6) with respect to the strains. However, the operator $\mathcal{G}\delta\mathbf{L}$ there does not always possess the needed symmetry (with respect to the external pairs of indices). Therefore it is not, in general, a self-adjoint operator in the space of second-rank symmetric tensor fields and thus *cannot* be replaced by a variational principle of the kind of (4.1). Hence the introduction of the polarization field $\boldsymbol{\tau}(\mathbf{x})$ instead of strain $\boldsymbol{\varepsilon}(\mathbf{x})$, see (2.14), is not a certain formal manipulation, but a simple and natural way to recast (2.6) into an equation with a self-adjoint operator [see Eqs. (2.13)], *whatever* the elastic tensors of the constituents and the symmetry of their arrangement.

3. Consider the case when the spatial distribution is one and the same for all inclusion pairs

$$\mathbf{P}_{\mathrm{d}}^{(rs)} \equiv \mathbf{P}_{\mathrm{d}} \quad \text{for} \quad r, s = 2, \ldots, N. \tag{5.1}$$

Then simple and meaningful bounds on the effective moduli can be extracted from (4.3), discussed in detail by Ponte Castañeda and Willis (1995). It is remarked here that in this (and only in this) case the solution of (4.3) has the form

$$\boldsymbol{\varepsilon}^{(r)} = \mathbf{A}^{(r)}\boldsymbol{\varepsilon}_{\mathrm{eff}}, \tag{5.2}$$

where

$$\boldsymbol{\varepsilon}_{\mathrm{eff}} = \left[\mathbf{I} - \mathbf{P}_{\mathrm{d}} \sum_{s=2}^{N} c^{(s)} \delta\mathbf{L}^{(s)} \mathbf{A}^{(s)} \right]^{-1} \boldsymbol{\varepsilon}_0, \tag{5.3}$$

and $\mathbf{A}^{(r)}$ are the single-ellipsoid tensors, defined in Eq. (2.15). The interpretation of Eq. (5.2) is obvious. It means that there exists a certain common and constant effective field $\boldsymbol{\varepsilon}_{\mathrm{eff}}$, explicitly given in Eq. (5.3), acting on each inclusion. Since the latter are differently oriented and possess different properties, the strain (and hence polarization), induced within them by the field $\boldsymbol{\varepsilon}_{\text{eff}}$ will be different as well.

4. Consider finally the case when only one family of aligned ellipsoidal particles exists in the matrix ($N = 2$). Recall that the well-known approximation of Mori-Tanaka (1973) for such a two-phase medium corresponds to the assumption that the particles are embedded into an effective field that coincides with the mean strain in the matrix:

$$\boldsymbol{\varepsilon}_{\text{eff}} = \langle\boldsymbol{\varepsilon}\rangle_1, \quad \text{i.e.} \quad \langle\boldsymbol{\varepsilon}\rangle_2 = \mathbf{A}^{(2)}\langle\boldsymbol{\varepsilon}\rangle_1\,, \tag{5.4}$$

see Benveniste (1987). But for an arbitrary two-phase medium

$$c^{(1)}\langle\boldsymbol{\varepsilon}\rangle_1 + c^{(2)}\langle\boldsymbol{\varepsilon}\rangle_2 = \boldsymbol{\varepsilon}_0$$

which, together with Eq. (5.4) gives

$$\boldsymbol{\varepsilon}_{\text{eff}} = \left[\, c^{(1)}\mathbf{I} + c^{(2)}\mathbf{A}^{(2)}\,\right]^{-1}\boldsymbol{\varepsilon}_0. \tag{5.5}$$

Simple check, based on the formula (2.15) for $\mathbf{A}^{(2)}$, shows that the expression (5.5) for the effective field coincides with the formula (5.3) for $\boldsymbol{\varepsilon}_{\text{eff}}$ (at $N = 2$) only if

$$\mathbf{P}_{\mathrm{i}}^{(2)} = \mathbf{P}_{\mathrm{d}}, \tag{5.6}$$

i.e. if the (ellipsoidal) symmetry of the inclusions and of their spatial distribution coincide. Hence this is the only case when the Mori-Tanaka approximation, for the binary medium under study, provides a rigorous Hashin-Shtrikman estimate on the effective elastic moduli. Note that the condition (5.6) obviously holds for a dispersion of spheres, isotropically distributed throughout a matrix. One then recovers the well-known fact that Mori-Tanaka's approximation in this case is just the appropriate Hashin-Shtrikman bound on the elastic moduli of such a dispersion.

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