A differential approach to microstructure-dependent bounds for multiphase heterogeneous media

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Abstract

We present a new method of deriving microstructure-dependent bounds on the effective properties of general heterogeneous media. The microstructure is specified by the average Eshelby tensors. In the small contrast limit, we introduce and calculate the expansion coefficient tensors. We then show that the effective tensor satisfies a differential inequality with the initial condition given by the expansion coefficient tensors in the small contrast limit. Using the comparison theorem we obtain rigorous bounds on the effective tensors of multiphase composites. These new bounds, taking into account of the average Eshelby tensors for homogeneous problems, are much tighter than the microstructure-independent Hashin-Shtrikman bounds. Also, these bounds are applicable to non-well-ordered composites and multifunctional composites. We anticipate that this new approach will be useful for the modeling and optimal design of multiphase multifunctional composites.

1 Introduction

In the theories of composite materials, fracture mechanics, dislocations and solid phase transformations, two problems appear often: the first is to evaluate the elastic energy arising from the presence of inhomogeneities for a given microstructure; the second is to find the microstructure of the inhomogeneities minimizing the energy under some constraint, e.g., a fixed volume fraction. The solution to the first problem is generally straightforward, at least numerically; the practical difficulty arises from the multiple scales of inhomogeneities and/or the singularities of the fields associated with singular geometries or high-contrast of material properties. The second problem is much more difficult and usually attacked by the indirect method of first deriving microstructure-independent bounds on the energy, and then constructing a microstructure to attain the bounds.

The importance of the above problems cannot be overstated, as evident in the two most cited papers in the area of solid mechanics, which are Eshelby (1957 [16]) and Mori-Tananka (1973 [34]). The closed-form solutions due to Eshelby for ellipsoidal inclusions have played a central role in the development of many, if not all, models about heterogeneous media. Reasons for the ubiquitous use of the Eshelby's solutions include that (i) Ellipsoids have the right geometrical complexity. They are simple and the geometric parameters can be easily measured and determined by volume, orientation, and aspect ratios. (ii) Important singular geometries such as cracks and fibers can be regarded as the limits of ellipsoids. (iii) Eshelby's solutions are closed-form. Physically important quantities such as energy, strain and stress fields in the inclusion are explicitly given, and predictions based on the Eshelby's solutions can usually be obtained by simply solving algebraic equations, which can then be compared with the experiments.

In his celebrated paper of 1957, Eshelby initially solved the homogeneous problem with a uniform eigenstrain on a subdomain called inclusion. In applying his solutions for homogeneous media to inhomogeneous problems where material properties on the inclusion are different from the matrix, he observed a remarkable property of ellipsoids: the induced strain is uniform on the ellipsoidal inclusion. By this, now called the *Eshelby uniformity property*, and some simple algebraic argument, Eshelby (1957) showed that his solutions for a homogeneous inclusion are also solutions for an inhomogeneous inclusion, provided that the eigenstrain is chosen appropriately — This is the so-called *equivalent inclusion method* [36, 37]. However, two or more ellipsoids together do not enjoy the Eshelby uniformity property, and the equivalent inclusion method cannot be used to solve the inhomogeneous problem when interactions between inhomogeneities are important, e.g., two cracks near to each other and composites with a non-dilute volume fraction of inhomogeneities. To overcome the limitation of the analysis based on the Eshelby's solutions, a prevailing approximation scheme, referred to as the Mori-Tanaka theory [34], is often employed. In this approach, the "concentration tensors" [48] that maps the average perturbed strain (stress) in the matrix phase to the average perturbed strain (stress) in the inclusion phase, though unknown for inhomogeneous media with a nontrivial volume fraction, are nevertheless replaced by the inhomogeneous media in the dilute limit where the Eshelby's single inclusion model is applicable [6]. Therefore, the final problem in this approach amounts to evaluating the average Eshelby tensors on the inclusions in the dilute limit, which are further approximated by solving the homogeneous inclusion problem. In addition, Weng (1990 [49]) showed that the predictions based on the Mori-Tanaka method always lie in the rigorous Hashin-Shtrikman-Walpole bounds and hence placed the method on a firm theoretical ground. Advantages of this approach lie in the closed-form predictions of the effective tensors of the media and can be conveniently compared with experiments.

Like any closed-form *effective medium theories* [16, 34, 7, 39], the constitutive models based on analytically solvable microstructures are inherently approximate since the microstructures of real-world composites can never be exactly the microstructures assumed in the models and are often too complicated to be described in precise geometric terms. A different but related approach to the effective properties of multiphase composites, particularly advocated by Hashin, is to derive *rigorous and microstructure-independent* bounds on the effective properties of composites. Hashin (1970 [22]) has argued that, since closed-form predictions of the energy or the effective properties of composites are inherently nonrigorous, rigorous microstructure-independent bounds shall be used whenever they are available. This philosophy has motivated many authors to derive rigorous bounds and construct optimal microstructures for two-phase and multiphase composites in various physical settings including elasticity [43, 5], conductivity [10, 18, 1, 11], cross-property [12, 19, 46, 13] among others [31]. The methods of deriving bounds include the classic the Hashin-Shtrikman method [23, 24, 32, 2] and the compensated compactness or translation method [44, 28, 38, 31]. The optimal microstructures include the Hashin's construction of coated spheres [21], Milton's construction of coated ellipsoids [30], multi-rank laminates [29], the Vigdergauz microstructures [47, 20] and recently found periodic E-inclusions [27, 26]. The advantage of this approach obviously lies in its rigor and generality. The disadvantage, as Berryman (1980 [7]) has pointed out, is that microstructure-independent bounds completely ignore our knowledge on the microstructure even if it is available from experimental observations. Also, the bounds are often far apart in cases of most interest. For applications and comparisons with experiments, it is certainly more desirable to have closed-form predictions. Another technical issue associated with this approach is the assumed "well-ordered" condition, i.e., the difference of the two tensors describing the material properties are either positive semi-definite or negative semi-definite. Neither the method based on the Hashin-

Shtrikman variational principle and nor the translation method yields optimal bounds for generic non-well-ordered cases.

Following the above influential works, particularly, Eshelby (1957, 1961), Hashin & Shtrikman (1962a, 1962b, 1963), Walpole (1966), Mori & Tanaka (1973), Bevinite (1987), Weng (1990), Milton (2002) and references therein, we may raise the following questions: (i) To what extent, the formulas predicted by the Mori-Tanaka theory are accurate enough for practical applications? (ii) Can we find some rigorous bounds while taking into account the observed microstructure through, e.g., the average Eshelby tensors for the homogeneous problem? (iii) What are the attaining microstructures for these bounds? and (iv) What are the optimal bounds for non-well-ordered cases?

In an attempt to answer the above the questions, we propose a new approach to deriving bounds for multiphase composites. We remark that the method is general and can be used to address physical problems including elasticity, conductivity, cross-property among others, though the motivation of this work originates from problems in elasticity and terminologies such as stress, strain, and stiffness and compliance tensors are employed for the purpose of bookkeeping. The obtained bounds, on one hand, are microstructure-dependent and expressed in parameters including the average Eshelby tensors, and on the other hand, can recover the classic microstructure-independent Hashin-Shtrikman bounds upon solving an algebraic maximization problem over the possible average Eshelby tensors. Also, the bounds do not require well-ordered conditions and apply to general anisotropic materials.

Heuristically, the idea is as follows. Let $\mathbf{L}(\mathbf{x},t)$ be the media interpolating a homogeneous comparison medium $\mathbf{L}_c$ and the inhomogeneous medium $\mathbf{L}_*(\mathbf{x})$ as the parameter t varies between zero and one, and $\mathbf{L}^e(t)$ be the associated effective stiffness tensor. Differentiating $\mathbf{L}^e(t)$ with respect to t, we may establish an identity

$$\frac{d}{dt}\mathbf{L}^e = F(\mathbf{L}^e, t), \tag{1.1}$$

where F is some function. We recognize the above equation describes *a flow* in the symmetric tensor space $\mathbb{L}_{\rm sym} := \{\mathbf{L} : \mathbb{R}^{m\times n} \to \mathbb{R}^{m\times n} \text{ is symmetric}\}$. In general, the function $F(\mathbf{L}^e, t)$ is unknown and depends on the microstructure, but a bound on $F(\mathbf{L}^e, t)$, e.g., $F(\mathbf{L}^e, t) \le F_0(\mathbf{L}^e, t)$, can be found by using quasiconvex functions and solving algebraic minimization problems. From this bound, we have

$$\frac{d}{dt}\mathbf{L}^e \le F_0(\mathbf{L}^e, t). \tag{1.2}$$

Further, we solve explicitly the ordinary differential system

$$\frac{d}{dt}\mathbf{L}^e_0 = F_0(\mathbf{L}^e_0, t). \tag{1.3}$$

Then an application of the comparison theorem to (1.2)-(1.3) yields bounds on $\mathbf{L}^e(t)$ in terms of $\mathbf{L}^e_0(t)$ and the initial conditions at $t \to 0$. The initial conditions at $t \to 0$ are provided by perturbation calculations and in particular, related with the average Eshelby tensors. Similar argument can be applied to the effective compliant tensor $\mathbf{M}^e(t)$ yielding the "dual" bounds.

We remark that the use of differential schemes in the modeling of composite materials has been an area of significant activity. With respect to volume fraction, the differential scheme has been used by Bruggerman (1935) and Norris (1985) and proven to be realizable by Milton (1985). Norris *et al.* (1985) also applies this scheme to suspensions of inclusions of a wide variety of shapes which have been proved to be realizable by Avellaneda (1987). Lipton (1993) develops optimal inequalities for polarization and Eshelby tensors to obtain useful differential inequalities. Compared to these works, the present work consider differential scheme with respect to “contrast” instead of volume fraction and the microstructure is characterized by the average Eshelby tensor instead of the actual geometries of inhomogeneities.

The paper is organized as follows. In § 2 by Fourier analysis we present general formulas for computing lower bounds of the energy of gradient fields $\mathbb{G}$ and divergence-free fields $\mathbb{P}$ in a homogeneous comparison medium. These lower bounds are useful for deriving the inequality (1.2). In § 3-4 we derive the bounds on the effective tensors and the attainment conditions for these bounds. In § 5 we compute the average Eshelby tensors and relate them with the expansion coefficient tensors. We summarize and present an outlook of possible applications in § 6.

Notation. We consider $(N+1)$-phase composites in n-dimensional space. Without loss of generality assume that the composite is periodic with an open bounded unit cell Y of volume one, e.g., $(0,1)^n$. In other words, the unit cell Y is a representive volume element (RVE) of the composite. Denote by $\theta_\alpha \in (0,1)$ the volume fraction of phase-α.

We will consider generic fields that take values from $\mathbb{R}^{m\times n}$, where m is a positive integer. For brevity denote $\mathbb{R}^{m\times n}$ by $\mathbb{U}$; the inner product of $\mathbf{F}_1, \mathbf{F}_2 \in \mathbb{U}$, is defined as $\mathbf{F}_1 \cdot \mathbf{F}_2 = \mathrm{Tr}(\mathbf{F}_1^T \mathbf{F}_2)$. Let $\mathbb{L}$ be the tensor space of all linear mappings $\mathbf{L} : \mathbb{U} \to \mathbb{U}$, and $\mathbb{L}_{\mathrm{sym}}$ be the subspace of symmetric tensors satisfying $\mathbf{F}_1 \cdot \mathbf{L}\mathbf{F}_2 = \mathbf{F}_2 \cdot \mathbf{L}\mathbf{F}_1$ for all $\mathbf{F}_1, \mathbf{F}_2 \in \mathbb{U}$. In index form the operation of a tensor $\mathbf{L} \in \mathbb{L}$ on a matrix $\mathbf{F} \in \mathbb{U}$ can be represented as

$$(\mathbf{L}\mathbf{F})_{pi} = (\mathbf{L})_{piqj}(\mathbf{F})_{qj},$$

where $p,q = 1,\cdots,m$; $i,j = 1,\cdots,n$, and repeated indices imply summation. For two tensors $\mathbf{L}_1, \mathbf{L}_2$, by $\mathbf{L}_1 > (\geq)\mathbf{L}_2$ we mean $\mathbf{L}_1 - \mathbf{L}_2$ is positive definite (positive semi-definite). The meanings of $\mathbf{L}_1 < (\leq)\mathbf{L}_2$ are likewise. Denote by $\mathbb{L}^+_{\mathrm{sym}} = \{\mathbf{L} \in \mathbb{L}_{\mathrm{sym}} : \mathbf{L} > 0\}$, $\overline{\mathbb{L}^+_{sym}} = \{\mathbf{L} \in \mathbb{L}_{\mathrm{sym}} : \mathbf{L} \geq 0\}$, and $\mathbb{L}^+_{\mathrm{ellip}} = \{\mathbf{L} \in \mathbb{L}_{\mathrm{sym}} : (\mathbf{a}\otimes\mathbf{b}) \cdot \mathbf{L}(\mathbf{a}\otimes\mathbf{b}) > c|\mathbf{a}|^2|\mathbf{b}|^2 \text{ for some } c > 0\ \forall\, \mathbf{a} \in \mathbb{R}^m, \mathbf{b} \in \mathbb{R}^n\}$ be the subset of strictly elliptic tensors. Note that $\mathbb{L}^+_{\mathrm{sym}} \subset \mathbb{L}^+_{\mathrm{ellip}}$ and the inclusion is strict if $m,n > 1$.

Further, we denote by $L^2(Y;\mathbb{U})$ the space of all square integrable functions $\boldsymbol{\phi} : Y \to \mathbb{U}$. For any $\boldsymbol{\phi} \in L^2(Y;\mathbb{U})$, by Fourier transformation we have

$$\boldsymbol{\phi}(\mathbf{x}) = \hat{\boldsymbol{\phi}}_0 + \sum_{\mathbf{k}\in\mathcal{K}} \hat{\boldsymbol{\phi}}_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{x}), \qquad \hat{\boldsymbol{\phi}}_{\mathbf{k}} = \fint_Y \boldsymbol{\phi}(\mathbf{x}) \exp(-i\mathbf{k}\cdot\mathbf{x}). \tag{1.4}$$

Here and subsequently, $\mathcal{L}$ is the Bravais lattice associated with the unit cell Y, $\mathcal{K}$ is the reciprocal lattice with the point zero removed, and $\fint_V$ denotes the average value of the integrand over the domain V. Let

$$\begin{aligned} \mathbf{g}(\mathbf{x}) &= \sum_{\mathbf{k}\in\mathcal{K}} \hat{\mathbf{g}}_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{x}), \qquad \hat{\mathbf{g}}_{\mathbf{k}} = (\hat{\boldsymbol{\phi}}_{\mathbf{k}}\hat{\mathbf{k}}) \otimes \hat{\mathbf{k}}, \\ \boldsymbol{\sigma}(\mathbf{x}) &= \sum_{\mathbf{k}\in\mathcal{K}} \hat{\boldsymbol{\sigma}}_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{x}), \qquad \hat{\boldsymbol{\sigma}}_{\mathbf{k}} = \hat{\boldsymbol{\phi}}_{\mathbf{k}} - (\hat{\boldsymbol{\phi}}_{\mathbf{k}}\hat{\mathbf{k}}) \otimes \hat{\mathbf{k}}, \end{aligned} \tag{1.5}$$

where $\hat{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$. The symbol $\mathbf{g}$ stands for “gradient”; $\boldsymbol{\sigma}$ is the usual notation for stress which is divergence free (in equilibrium and no body force). We therefore obtain the following orthogonal decomposition:

$$\begin{aligned} &\boldsymbol{\phi} = \hat{\boldsymbol{\phi}}_0 + \mathbf{g} + \boldsymbol{\sigma}, \\ &\fint_Y \mathbf{g}\cdot\boldsymbol{\sigma} = \fint_Y \mathbf{g}\cdot\hat{\boldsymbol{\phi}}_0 = \fint_Y \boldsymbol{\sigma}\cdot\hat{\boldsymbol{\phi}}_0 = 0. \end{aligned} \tag{1.6}$$

We remark that the above decomposition is unique and we denote by $\mathbb{G}$ and $\mathbb{P}$ the collection of all such $\mathbf{g}$ and $\boldsymbol{\sigma}$. In real space, these function spaces are identified as:

$$\mathbb{G} = \{\mathbf{g} \in L^2(Y;\mathbb{U}) : \mathbf{g} = \nabla \mathbf{u},\ \mathbf{u} = \sum_{\mathbf{k}\in\mathcal{K}} \hat{\mathbf{u}}_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{x}) \text{ for some } \hat{\mathbf{u}}_{\mathbf{k}} \in \mathbb{C}^m\},$$
$$\mathbb{P} = \{\boldsymbol{\sigma} \in L^2(Y;\mathbb{U}) : \mathrm{div}\boldsymbol{\sigma} = 0,\ \ \boldsymbol{\sigma} = \sum_{\mathbf{k}\in\mathcal{K}} \hat{\boldsymbol{\sigma}}_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{x}) \text{ for some } \hat{\boldsymbol{\sigma}}_{\mathbf{k}} \in \mathbb{C}^{m\times n}\},$$

where the pth row vector of $\nabla\mathbf{u}$ is the gradient of the pth component of $\mathbf{u}$ and the "div" operates on the row vectors. In the case $m = n$, a subspace of $\mathbb{G}$ is obtained by taking the second gradient of the scalar functions in

$$\mathbb{W} = \{\xi :\ \nabla\nabla\xi \in \mathbb{G},\ \xi = \sum_{\mathbf{k}\in\mathcal{K}} \hat{\xi}_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{x}) \text{ for some } \hat{\xi}_{\mathbf{k}} \in \mathbb{C}\}.$$

2 Quasiconvexity inequalities

In the two classic methods of deriving energy bounds for inhomogeneous media, i.e., the Hashin-Shtrikman's method and the compensated compactness or translation method, it is necessary to have a priori estimates on energy of the field in a homogeneous comparison medium. In the Hashin-Shtrikman's approach and in terms of homogeneous Eshelby inclusion problems, this is hidden in the Bitter-Crum theorem which states that the strain energy associated with an dilatational eigenstress in an isotropic medium depends only on the volume (fraction) of the inclusions. In the compensated compactness or translation method, we directly use the inequality

$$\fint_Y W(\mathbf{g}) \geq W(0) \qquad \forall\, \mathbf{g} \in \mathbb{G}, \tag{2.1}$$

where the usual choice of the function $W : \mathbb{U} \to \mathbb{R}$ is the determinant or some linear combination of subdeterminants (Ericksen 1962 [15]). In a more general setting, equalities or inequalities of the above type arise from the quasiconvexity of the function W (Morrey, 1952; Ball, 1977). We remark that quasiconvex functions, though originally defined for gradient fields, can be similarly defined for fields with other differential constraints, e.g., divergence-free fields in $\mathbb{P}$ (Tartar, 1985).

For energy bounds on linear inhomogeneous media, quadratic quasiconvex functions are particularly useful. The following lemma gives explicit formulas to calculate general quadratic quasiconvex functions with respect to gradient fields in $\mathbb{G}$ and divergence-free fields in $\mathbb{P}$.

Lemma 1 *Let $\mathbf{L} \in \mathbb{L}^+_{\mathrm{ellip}}$ be a strictly elliptic tensor, $\mathbf{E} \in \mathbb{U}$ be a nonzero matrix, $\hat{\mathbf{k}} \in \mathbb{R}^n$ be unit vectors, $\mathbf{N}$ be the inverse of the matrix $(\mathbf{L})_{piqj}(\hat{\mathbf{k}})_i(\hat{\mathbf{k}})_j$, and $\boldsymbol{\omega} = (\mathbf{L}\mathbf{E})\hat{\mathbf{k}} \in \mathbb{R}^m$. (Note that the matrix $\mathbf{N}$ and the vector $\boldsymbol{\omega}$ depend on the unit vector $\hat{\mathbf{k}}$.) Denote by*

$$\rho_{\mathbf{g}}(\mathbf{L},\mathbf{E}) = \min_{|\hat{\mathbf{k}}|=1} \frac{1}{\hat{\mathbf{k}}\cdot\mathbf{E}^T\mathbf{N}\mathbf{E}\hat{\mathbf{k}}}\ , \tag{2.2}$$

$$\rho_{\boldsymbol{\sigma}}(\mathbf{L},\mathbf{E}) = \min_{|\hat{\mathbf{k}}|=1} \frac{1}{[\mathbf{E}-(\mathbf{N}\boldsymbol{\omega})\otimes\hat{\mathbf{k}}]\cdot\mathbf{L}[\mathbf{E}-(\mathbf{N}\boldsymbol{\omega})\otimes\hat{\mathbf{k}}]}\ , \tag{2.3}$$

$$\mathcal{S}_{\mathbf{g}}(\mathbf{L},\mathbf{E}) = \Big\{c\hat{\mathbf{k}} :\ c\in\mathbb{R},\ \frac{1}{\hat{\mathbf{k}}\cdot\mathbf{E}^T\mathbf{N}\mathbf{E}\hat{\mathbf{k}}} = \rho_{\mathbf{g}}(\mathbf{L},\mathbf{E})\Big\}, \tag{2.4}$$

and

$$\mathcal{S}_{\boldsymbol{\sigma}}(\mathbf{L},\mathbf{E})=\Big\{c\hat{\mathbf{k}}:\ c\in\mathbb{R},\ \frac{1}{[\mathbf{E}-(\mathbf{N}\boldsymbol{\omega})\otimes\hat{\mathbf{k}}]\cdot\mathbf{L}[\mathbf{E}-(\mathbf{N}\boldsymbol{\omega})\otimes\hat{\mathbf{k}}]}=\rho_{\boldsymbol{\sigma}}(\mathbf{L},\mathbf{E})\Big\}. \tag{2.5}$$

(i) For any $\mathbf{g}\in\mathbb{G}$*,*

$$⨍_Y \mathbf{g}\cdot\mathbf{L}\mathbf{g}\geq\rho_{\mathbf{g}}(\mathbf{L},\mathbf{E})⨍_Y|\mathbf{g}\cdot\mathbf{E}|^2, \tag{2.6}$$

where equality holds if and only if for some $c_{\mathbf{k}}\in\mathbb{C}$*,*

$$\mathbf{g}(\mathbf{x})=\sum_{\mathbf{k}\in\mathcal{K}\cap\mathcal{S}_{\mathbf{g}}(\mathbf{L},\mathbf{E})}\hat{\mathbf{u}}_{\mathbf{k}}\otimes\hat{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{x}),\qquad \hat{\mathbf{u}}_{\mathbf{k}}=c_{\mathbf{k}}\mathbf{N}\mathbf{E}\hat{\mathbf{k}}. \tag{2.7}$$

(ii) For any $\boldsymbol{\sigma}\in\mathbb{P}$*,*

$$⨍_Y \boldsymbol{\sigma}\cdot\mathbf{L}^{-1}\boldsymbol{\sigma}\geq\rho_{\boldsymbol{\sigma}}(\mathbf{L},\mathbf{E})⨍_Y|\boldsymbol{\sigma}\cdot\mathbf{E}|^2, \tag{2.8}$$

where equality holds if and only if for some $c_{\mathbf{k}}\in\mathbb{C}$*,*

$$\boldsymbol{\sigma}(\mathbf{x})=\sum_{\mathbf{k}\in\mathcal{K}\cap\mathcal{S}_{\boldsymbol{\sigma}}(\mathbf{L},\mathbf{E})}\hat{\boldsymbol{\sigma}}_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{x}),\qquad \hat{\boldsymbol{\sigma}}_{\mathbf{k}}=c_{\mathbf{k}}[\mathbf{L}\mathbf{E}-\mathbf{L}(\mathbf{N}\boldsymbol{\omega})\otimes\hat{\mathbf{k}}]. \tag{2.9}$$

Proof: From (1.5), for any $\mathbf{g}\in\mathbb{G}$ the Fourier coefficients $\hat{\mathbf{g}}(\mathbf{k})$ satisfy that for some $\hat{\mathbf{u}}_{\mathbf{k}}\in\mathbb{C}^m$,

$$\hat{\mathbf{g}}(\mathbf{k})=\hat{\mathbf{u}}_{\mathbf{k}}\otimes\hat{\mathbf{k}}. \tag{2.10}$$

From the Parseval's theorem (Rudin 1987), we have

$$⨍_Y \mathbf{g}\cdot\mathbf{L}\mathbf{g}=\sum_{\mathbf{k}\in\mathcal{K}}(\hat{\mathbf{u}}_{\mathbf{k}}^*\otimes\hat{\mathbf{k}})\cdot\mathbf{L}(\hat{\mathbf{u}}_{\mathbf{k}}\otimes\hat{\mathbf{k}}), \tag{2.11}$$

and

$$⨍_Y|\mathbf{g}\cdot\mathbf{E}|^2=\sum_{\mathbf{k}\in\mathcal{K}}|\mathbf{u}_{\mathbf{k}}\cdot\mathbf{E}\hat{\mathbf{k}}|^2. \tag{2.12}$$

Consider the algebraic minimization problem

$$m_{\mathbf{g}}(\hat{\mathbf{k}}):=\min\{(\mathbf{a}^*\otimes\hat{\mathbf{k}})\cdot\mathbf{L}(\mathbf{a}\otimes\hat{\mathbf{k}}):\ \mathbf{a}\cdot\mathbf{E}\hat{\mathbf{k}}=\lambda,\ \mathbf{a}\in\mathbb{C}^m\}.$$

By the method of Lagrangian multiplier, we find the minimum is given by

$$m_{\mathbf{g}}(\hat{\mathbf{k}})=\frac{|\lambda|^2}{\hat{\mathbf{k}}\cdot\mathbf{E}^T\mathbf{N}\mathbf{E}\hat{\mathbf{k}}}, \tag{2.13}$$

and the minimum is attained if and only if for some $c\in\mathbb{C}$,

$$\mathbf{a}=c\mathbf{N}\mathbf{E}\hat{\mathbf{k}}. \tag{2.14}$$

Further, from (2.2) and (2.13) we see that

$$(\mathbf{a}^*\otimes\hat{\mathbf{k}})\cdot\mathbf{L}(\mathbf{a}\otimes\hat{\mathbf{k}})\geq\rho_{\mathbf{g}}(\mathbf{L},\mathbf{E})|\mathbf{a}\cdot\mathbf{E}\hat{\mathbf{k}}|^2\qquad\forall\,|\hat{\mathbf{k}}|=1\,\&\,\mathbf{a}\in\mathbb{C}^m. \tag{2.15}$$

Additionally, by (2.4) and (2.14) equality holds for (2.15) if and only if for some $c \in \mathbb{C}$,

$$\mathbf{a} = c\mathbf{N}\mathbf{E}\hat{\mathbf{k}} \qquad \text{and} \qquad \hat{\mathbf{k}} \in \mathcal{S}_{\mathbf{g}}(\mathbf{L}, \mathbf{E}).$$

Therefore, by (2.11), (2.12) and (2.15) we have

$$\fint_Y \mathbf{g} \cdot \mathbf{L}\mathbf{g} = \sum_{\mathbf{k}\in\mathcal{K}} (\hat{\mathbf{u}}^*_{\mathbf{k}} \otimes \hat{\mathbf{k}}) \cdot \mathbf{L}(\hat{\mathbf{u}}_{\mathbf{k}} \otimes \hat{\mathbf{k}}) \geq \rho_{\mathbf{g}}(\mathbf{L}, \mathbf{E}) \sum_{\mathbf{k}\in\mathcal{K}} |\hat{\mathbf{u}}_{\mathbf{k}} \cdot \mathbf{E}\hat{\mathbf{k}}|^2 = \rho_{\mathbf{g}}(\mathbf{L}, \mathbf{E}) \fint_Y |\mathbf{g} \cdot \mathbf{E}|^2,$$

which completes the proof of (2.6) and the attainment condition (2.7). Below we show part (ii) of the lemma.

From (1.5), for any $\boldsymbol{\sigma} \in \mathbb{P}$ the Fourier coefficients $\hat{\boldsymbol{\sigma}}(\mathbf{k})$ satisfy that

$$\hat{\boldsymbol{\sigma}}(\mathbf{k})\hat{\mathbf{k}} = 0 \qquad \forall\, \mathbf{k} \in \mathcal{K}. \tag{2.16}$$

By the Parseval's theorem we obtain

$$\fint_Y \boldsymbol{\sigma} \cdot \mathbf{L}^{-1}\boldsymbol{\sigma} = \sum_{\mathbf{k}\in\mathcal{K}} \hat{\boldsymbol{\sigma}}^*_{\mathbf{k}} \cdot \mathbf{L}^{-1}\hat{\boldsymbol{\sigma}}_{\mathbf{k}}, \tag{2.17}$$

and

$$\fint_Y |\boldsymbol{\sigma} \cdot \mathbf{E}|^2 = \sum_{\mathbf{k}\in\mathcal{K}} |\hat{\boldsymbol{\sigma}}_{\mathbf{k}} \cdot \mathbf{E}|^2. \tag{2.18}$$

Consider the algebraic minimization problem

$$m_{\boldsymbol{\sigma}}(\hat{\mathbf{k}}) := \min\{\boldsymbol{\pi}^* \cdot \mathbf{L}^{-1}\boldsymbol{\pi} :\ \boldsymbol{\pi} \in \mathbb{C}^{m\times n},\ \boldsymbol{\pi}\hat{\mathbf{k}} = 0,\ \boldsymbol{\pi} \cdot \mathbf{E} = \lambda'\}.$$

By the method of Lagrangian multiplier, we find that a minimizer $\boldsymbol{\pi}$ to the above problem necessarily satisfies that for some $c_0 \in \mathbb{C}$ and $\mathbf{d} \in \mathbb{C}^m$,

$$\boldsymbol{\pi} = c_0\mathbf{L}\mathbf{E} + \mathbf{L}(\mathbf{d} \otimes \hat{\mathbf{k}}).$$

From the constraints $\boldsymbol{\pi}\hat{\mathbf{k}} = 0$ and $\boldsymbol{\pi} \cdot \mathbf{E} = \lambda'$, we find that $\mathbf{d} = -c_0\mathbf{N}\boldsymbol{\omega}$ (recall that $\boldsymbol{\omega} = (\mathbf{L}\mathbf{E})\hat{\mathbf{k}}$),

$$c_0 = \frac{\lambda'}{\mathbf{E} \cdot \mathbf{L}\mathbf{E} - \boldsymbol{\omega} \cdot \mathbf{N}\boldsymbol{\omega}} = \frac{\lambda'}{[\mathbf{E} - (\mathbf{N}\boldsymbol{\omega}) \otimes \hat{\mathbf{k}}] \cdot \mathbf{L}[\mathbf{E} - (\mathbf{N}\boldsymbol{\omega}) \otimes \hat{\mathbf{k}}]}. \tag{2.19}$$

Thus, the minimum is given by

$$m_{\boldsymbol{\sigma}}(\hat{\mathbf{k}}) = \frac{|\lambda'|^2}{[\mathbf{E} - (\mathbf{N}\boldsymbol{\omega}) \otimes \hat{\mathbf{k}}] \cdot \mathbf{L}[\mathbf{E} - (\mathbf{N}\boldsymbol{\omega}) \otimes \hat{\mathbf{k}}]}, \tag{2.20}$$

and the minimum is attained if and only if for some $c \in \mathbb{C}$,

$$\boldsymbol{\pi} = c[\mathbf{L}\mathbf{E} - \mathbf{L}(\mathbf{N}\boldsymbol{\omega}) \otimes \hat{\mathbf{k}}]. \tag{2.21}$$

Further, from (2.3) and (2.20) we see that

$$\boldsymbol{\pi}^* \cdot \mathbf{L}^{-1}\boldsymbol{\pi} \geq \rho_{\mathbf{g}}(\mathbf{L}, \mathbf{E})|\boldsymbol{\pi} \cdot \mathbf{E}|^2 \qquad \forall\, \boldsymbol{\pi} \in \mathbb{U}. \tag{2.22}$$

Additionally, by (2.5) and (2.21) equality holds for (2.22) if and only if for some $c \in \mathbb{C}$,

$$\boldsymbol{\pi} = c[\mathbf{L}\mathbf{E} - \mathbf{L}(\mathbf{N}\boldsymbol{\omega}) \otimes \hat{\mathbf{k}}] \qquad \text{and} \qquad \hat{\mathbf{k}} \in \mathcal{S}_{\boldsymbol{\sigma}}(\mathbf{L}, \mathbf{E}).$$

Therefore, by (2.17), (2.18) and (2.22) we have

$$\fint_Y \boldsymbol{\sigma} \cdot \mathbf{L}^{-1}\boldsymbol{\sigma} = \sum_{\mathbf{k}\in\mathcal{K}} \boldsymbol{\sigma}^*_{\hat{\mathbf{k}}} \cdot \mathbf{L}^{-1}\boldsymbol{\sigma}_{\hat{\mathbf{k}}} \geq \rho_{\boldsymbol{\sigma}}(\mathbf{L}, \mathbf{E}) \sum_{\mathbf{k}\in\mathcal{K}} |\hat{\boldsymbol{\sigma}}_{\mathbf{k}} \cdot \mathbf{E}|^2 = \rho_{\boldsymbol{\sigma}}(\mathbf{L}, \mathbf{E}) \fint_Y |\boldsymbol{\sigma} \cdot \mathbf{E}|^2,$$

which completes the proof of (2.8) and the attainment condition (2.9).

■

3 Bounds on the effective stiffness tensors

3.1 Series expansions of the gradient fields and effective stiffness tensors

We first calculate the series expansions of the gradient fields and effective stiffness tensors by assuming the contrast of the composite is small. To some extent the calculation is classic, see e.g. Milton (2002, Chapter 14) and references therein. Our calculation extracts higher-order terms that explicitly depend on the average Eshelby tensor.

The inhomogeneous medium considered in this paper is specified by

$$\mathbf{L}_*(\mathbf{x}) = \mathbf{L}_\alpha \in \mathbb{L}^+_{\text{ellip}} \qquad \text{if } \mathbf{x} \in \Omega_\alpha,\ \alpha = 0, \cdots, N. \tag{3.1}$$

The periodic *inhomogeneous* Eshelby inclusion problem for a given applied average strain $\mathbf{F} \in \mathbb{U}$ is to find $\mathbf{g}_* \in \mathbb{G}$ such that

$$\mathbf{L}_*(\mathbf{x})(\mathbf{g}_* + \mathbf{F}) \in \mathbb{P} \oplus \mathbb{U}. \tag{3.2}$$

For many important applications, we need to calculate the energy

$$\mathcal{E}_*(\mathbf{F}) = \fint_Y [(\mathbf{g}_* + \mathbf{F}) \cdot \mathbf{L}_*(\mathbf{x})(\mathbf{g}_* + \mathbf{F})], \tag{3.3}$$

find how it depends on the microstructure and determine the optimal microstructure. Explicit closed-form solutions to the above problem are rare; we turn to the indirect method of first estimating the bounds on the energy and then constructing microstructures to attain these bounds. To this end, we propose a new method based on differential inequalities and comparison theorems for ordinary differential systems.

As in the method of Hashin-Shtrikman we first choose a homogeneous "comparison" medium $\mathbf{L}_c \in \mathbb{L}^+_{\text{ellip}}$. Let

$$\mathbf{L}(\mathbf{x}, t) = \mathbf{L}_c + t(\mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c) \in \mathbb{L}^+_{\text{ellip}} \qquad \forall\, t \in [0, 1] \tag{3.4}$$

interpolates between the homogeneous medium $\mathbf{L}_c$ and the heterogeneous medium $\mathbf{L}_*(\mathbf{x})$ as t varies in $[0, 1]$. For an average applied strain $\mathbf{F} \in \mathbb{U}$, we consider the minimization problem:

$$\mathcal{E}(\mathbf{F}, t) = \min_{\mathbf{g} \in \mathbb{G}} \fint_Y (\mathbf{g} + \mathbf{F}) \cdot \mathbf{L}(\mathbf{x}, t)(\mathbf{g} + \mathbf{F}). \tag{3.5}$$

The associated Euler-Lagrangian equation is to find $\mathbf{g}_t \in \mathbb{G}$ such that

$$\mathbf{L}(\mathbf{x}, t)(\mathbf{g}_t + \mathbf{F}) \in \mathbb{P} \oplus \mathbb{U}. \tag{3.6}$$

From equation (3.5), we verify that $\mathcal{E}(\mathbf{F}, t)$ is a quadratic function of $\mathbf{F}$, implying that there exists a symmetric tensor $\mathbf{L}^e(t) \in \mathbb{L}^+_{\text{ellip}}$ such that

$$\mathcal{E}(\mathbf{F}, t) = \mathbf{F} \cdot \mathbf{L}^e(t)\mathbf{F} \qquad \forall\, \mathbf{F} \in \mathbb{U}. \tag{3.7}$$

We remark that the tensor $\mathbf{L}^e(t)$ is precisely the effective tensor of the composite $\mathbf{L}(\mathbf{x}, t)$.

Clearly, if $t = 0$, the medium is homogeneous, a solution to (3.6) is trivially given by $\mathbf{g}_t\big|_{t=0} = 0$ and $\mathcal{E}(\mathbf{F}, 0) = \mathbf{F} \cdot \mathbf{L}_c\mathbf{F}$. Assume a small perturbation, i.e., $0 < |t| << 1$. It can be shown that the solutions to (3.6) can be written as

$$\mathbf{g}_t = t\mathbf{g}_1 + t^2\mathbf{g}_2 + t^3\mathbf{g}_3 + \cdots, \tag{3.8}$$

where $\mathbf{g}_i \in \mathbb{G}$ $(i = 1, 2, \cdots)$. Inserting the above expression into (3.6) and arranging terms according to the order of t, we rewrite (3.6) as

$$(\mathbf{L}_c + t(\mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c))(\mathbf{F} + t\mathbf{g}_1 + t^2\mathbf{g}_2 + t^3\mathbf{g}_3 + \cdots) \in \mathbb{P} \oplus \mathbb{U}, \tag{3.9}$$

and find that $\mathbf{g}_i \in \mathbb{G}$ necessarily satisfies

$$\begin{cases} \mathbf{L}_c\mathbf{g}_1 + (\mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c)\mathbf{F} \in \mathbb{P} \oplus \mathbb{U} & \text{if } i = 1, \\ \mathbf{L}_c\mathbf{g}_i + (\mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c)\mathbf{g}_{i-1} \in \mathbb{P} \oplus \mathbb{U} & \text{if } i > 1. \end{cases} \tag{3.10}$$

In particular, we notice that $(3.10)_1$ is equivalent to

$$\mathbf{L}_c\mathbf{g}_1 + (\mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c)\mathbf{F} = \mathbf{L}_c\mathbf{g}_1 + \sum_{\alpha=0}^{N} \triangle\mathbf{L}_\alpha\mathbf{F}\chi_\alpha \in \mathbb{P} \oplus \mathbb{U}, \tag{3.11}$$

where χ_α, equal to one on Ω_α and zero otherwise, is the characteristic function of domain Ω_α, and

$$\triangle\mathbf{L}_\alpha = \mathbf{L}_\alpha - \mathbf{L}_c \qquad \alpha = 0, \cdots, N. \tag{3.12}$$

As one will see below, the above problem is exactly the homogeneous Eshelby inclusion problem (5.2) with eigenstress $\mathbf{P}_\alpha = \triangle\mathbf{L}_\alpha\mathbf{F}$ on the inclusion Ω_α. By (3.7) and (3.8) we expand $\mathbf{L}^e(t)$ as a power series of t:

$$\mathbf{L}^e(t) = \sum_{i=0}^{\infty} t^i\mathbf{\Gamma}_i = \mathbf{\Gamma}_0 + t\mathbf{\Gamma}_1 + t^2\mathbf{\Gamma}_2 + t^3\mathbf{\Gamma}_3 + \cdots. \tag{3.13}$$

To find the expansion coefficient tensors $\mathbf{\Gamma}_i$, we differentiate (3.5) with respect to $\mathbf{F}$ and, by (3.7), (3.9) and (3.13), obtain

$$2\sum_{i=0}^{\infty} t^i\mathbf{\Gamma}_i\mathbf{F} = 2\mathbf{L}_c\mathbf{F} + 2t\left[\fint_Y \mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c\right]\mathbf{F} + 2t\fint_Y (\mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c)\mathbf{g}_t.$$

From the above equation, we immediately find that

$$\mathbf{\Gamma}_0 = \mathbf{L}_c, \qquad \mathbf{\Gamma}_1 = -\mathbf{L}_c + \fint_Y \mathbf{L}_*(\mathbf{x}), \tag{3.14}$$

and

$$\mathbf{\Gamma}_{i+1}\mathbf{F} = \fint_Y (\mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c)\mathbf{g}_i = \fint_Y \mathbf{L}_*(\mathbf{x})\mathbf{g}_i \qquad \text{if } i = 1, 2, \cdots. \tag{3.15}$$

Therefore,

$$(\mathbf{L}^e(t) - \mathbf{L}_c - t\mathbf{\Gamma}_1 - t^2\mathbf{\Gamma}_2)\mathbf{F} = \sum_{i=3}^{\infty} t^i\mathbf{\Gamma}_i\mathbf{F} = t\fint_Y (\mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c)(\mathbf{g}_t - t\mathbf{g}_1). \tag{3.16}$$

Further, by (3.15), $(3.10)_1$ and (1.6) we have

$$\mathbf{F} \cdot \mathbf{\Gamma}_2\mathbf{F} = \mathbf{F} \cdot \fint_Y (\mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c)\mathbf{g}_1 = -\fint_Y \mathbf{g}_1 \cdot \mathbf{L}_c\mathbf{g}_1. \tag{3.17}$$

Similarly, by (3.15), (3.10) and (1.6) we have

$$
\begin{aligned}
\mathbf{F}\cdot\boldsymbol{\Gamma}_3\mathbf{F} &= \fint_Y \mathbf{F}\cdot(\mathbf{L}_*(\mathbf{x})-\mathbf{L}_c)\mathbf{g}_2 = \fint_Y \mathbf{g}_2\cdot(\mathbf{L}_*(\mathbf{x})-\mathbf{L}_c)\mathbf{F} \\
&= -\fint_Y \mathbf{g}_2\cdot\mathbf{L}_c\mathbf{g}_1 = -\fint_Y \mathbf{g}_1\cdot\mathbf{L}_c\mathbf{g}_2 = \fint_Y \mathbf{g}_1\cdot(\mathbf{L}_*(\mathbf{x})-\mathbf{L}_c)\mathbf{g}_1,
\end{aligned}
\tag{3.18}
$$

The above equation indicates that the coefficient tensor $\boldsymbol{\Gamma}_3$ is completely determined by solving $(3.10)_1$ for $\mathbf{g}_1$. In general, we have the following theorem.

Theorem 2 *For any integer $i \geq 1$, let $\boldsymbol{\Gamma}_i$ be the expansion coefficient tensors satisfying (3.13) and $\mathbf{g}_i \in \mathbb{G}$ satisfy (3.10). Then*

$$
\begin{aligned}
&\fint_Y \mathbf{g}_i\cdot\mathbf{L}_c\mathbf{g}_j = -\mathbf{F}\cdot\boldsymbol{\Gamma}_{i+j}\mathbf{F}, \\
&\fint_Y \mathbf{g}_i\cdot(\mathbf{L}_*(\mathbf{x})-\mathbf{L}_c)\mathbf{g}_j = \mathbf{F}\cdot\boldsymbol{\Gamma}_{i+j+1}\mathbf{F},
\end{aligned}
\tag{3.19}
$$

We note that the above theorem implies that

$$
\begin{aligned}
&\mathbf{F}\cdot\boldsymbol{\Gamma}_{2i}\mathbf{F} = -\fint_Y \mathbf{g}_i\cdot\mathbf{L}_c\mathbf{g}_i, \\
&\mathbf{F}\cdot\boldsymbol{\Gamma}_{2i+1}\mathbf{F} = \fint_Y \mathbf{g}_i\cdot(\mathbf{L}_*(\mathbf{x})-\mathbf{L}_c)\mathbf{g}_i.
\end{aligned}
\tag{3.20}
$$

In other words, to determine the coefficient tensors $\boldsymbol{\Gamma}_0, \cdots, \boldsymbol{\Gamma}_{2i+1}$, it is sufficient to solve (3.10) for $\mathbf{g}_1, \cdots, \mathbf{g}_i$. This is quite useful for numerical calculations of higher order terms in the expansion (3.13) and appears to be unnoticed before.

Proof: By repeatedly using the argument in (3.18), for $i, j \geq 1$ we have

$$
\begin{aligned}
\fint_Y \mathbf{g}_i\cdot\mathbf{L}_c\mathbf{g}_j &= -\fint_Y \mathbf{g}_j\cdot(\mathbf{L}_*(\mathbf{x})-\mathbf{L}_c)\mathbf{g}_{i-1} = \fint_Y \mathbf{g}_{i-1}\cdot\mathbf{L}_c\mathbf{g}_{j+1} \\
&= \cdots = \fint_Y \mathbf{g}_1\cdot\mathbf{L}_c\mathbf{g}_{j+i-1} = -\mathbf{F}\cdot\fint(\mathbf{L}_*(\mathbf{x})-\mathbf{L}_c)\mathbf{g}_{j+i-1} \\
&= -\mathbf{F}\cdot\boldsymbol{\Gamma}_{i+j}\mathbf{F}.
\end{aligned}
$$

The other equation in (3.19) follows similarly.

■

We remark that the expansions (3.8) and (3.13) can be rigorously justified. In fact, the effective tensor $\mathbf{L}^e(t)$ is analytic on any open interval such that $\mathbf{L}(\mathbf{x}, t) \in \mathbb{L}^+_{\text{ellip}}$ for any $\mathbf{x} \in Y$. Further, the tensors $\boldsymbol{\Gamma}_2$ (resp. $\boldsymbol{\Gamma}_3$) may also be called (resp. higher-order) *polarization tensors*. This terminology originates from the works of Pólya-Szegö (1951 [41]). In particular, $\boldsymbol{\Gamma}_2$, upon a linear transformation and in various physical settings, can be identified as the demagnetization tensors in magnetics (Brown 1962 [8]), the (average) Eshelby tensors (Eshelby 1957 [16]) in linear elasticity, and the geometric parameter tensors in Firoozye and Kohn (1994) [17].

3.2 A differential identity

From (3.5) and (3.7), direct calculations reveal that

$$\frac{d}{dt}\mathcal{E}(\mathbf{F},t) = \mathbf{F}\cdot\frac{d\mathbf{L}^e(t)}{dt}\mathbf{F} = \fint_Y \Big\{(\mathbf{g}_t+\mathbf{F})\cdot(\mathbf{L}_*(\mathbf{x})-\mathbf{L}_c)(\mathbf{g}_t+\mathbf{F})\Big\} \\ +2\fint_Y \frac{d\mathbf{g}_t}{dt}\cdot[\mathbf{L}(\mathbf{x},t)(\mathbf{g}_t+\mathbf{F})]. \tag{3.21}$$

Clearly, $d\mathbf{g}_t/dt\in\mathbb{G}$ since $\mathbf{g}_t\in\mathbb{G}$ for all $t\in(0,1)$. Therefore, the last term on the right hand side of (3.21) vanishes by (3.6) and (1.6). By (3.4), (3.5) and (3.7), we rewrite the right hand side of the above equation as

$$\begin{aligned}&\fint_Y\Big\{\frac{1}{t}(\mathbf{g}_t+\mathbf{F})\cdot\mathbf{L}(\mathbf{x},t)(\mathbf{g}_t+\mathbf{F})-\frac{1}{t}(\mathbf{g}_t+\mathbf{F})\cdot\mathbf{L}_c(\mathbf{g}_t+\mathbf{F})\Big\}\\ &\qquad=\frac{1}{t}\Big[-\fint_Y\mathbf{g}_t\cdot\mathbf{L}_c\mathbf{g}_t+\mathbf{F}\cdot(\mathbf{L}^e(t)-\mathbf{L}_c)\mathbf{F}\Big].\end{aligned}\tag{3.22}$$

Thus, by (3.7), (3.21) and (3.22) we have that for any $t\in(0,1)$,

$$t\mathbf{F}\cdot\frac{d\mathbf{L}^e(t)}{dt}\mathbf{F} = -\fint_Y\mathbf{g}_t\cdot\mathbf{L}_c\mathbf{g}_t+\mathbf{F}\cdot(\mathbf{L}^e(t)-\mathbf{L}_c)\mathbf{F}. \tag{3.23}$$

Let

$$\mathbf{X}(t)=\mathbf{L}^e(t)-\mathbf{\Gamma}_0-t\mathbf{\Gamma}_1-t^2\mathbf{\Gamma}_2. \tag{3.24}$$

Then

$$\begin{aligned}\fint_Y\mathbf{g}_t\cdot\mathbf{L}_c\mathbf{g}_t &= \fint_Y(\mathbf{g}_t-t\mathbf{g}_1+t\mathbf{g}_1)\cdot\mathbf{L}_c(\mathbf{g}_t-t\mathbf{g}_1+t\mathbf{g}_1)\\ &=\fint_Y[t^2\mathbf{g}_1\cdot\mathbf{L}_c\mathbf{g}_1+2t\mathbf{g}_1\cdot\mathbf{L}_c(\mathbf{g}_t-t\mathbf{g}_1)+(\mathbf{g}_t-t\mathbf{g}_1)\cdot\mathbf{L}_c(\mathbf{g}_t-t\mathbf{g}_1)]\\ &=-t^2\mathbf{F}\cdot\mathbf{\Gamma}_2\mathbf{F}-2\mathbf{F}\cdot\mathbf{X}(t)\mathbf{F}+\fint_Y(\mathbf{g}_t-t\mathbf{g}_1)\cdot\mathbf{L}_c(\mathbf{g}_t-t\mathbf{g}_1),\end{aligned}\tag{3.25}$$

where for the last equality we have used (3.17) and, by (1.6), (3.11) and (3.16), the identity

$$\fint_Y\mathbf{g}_1\cdot\mathbf{L}_c(\mathbf{g}_t-t\mathbf{g}_1)=-\mathbf{F}\cdot\fint_Y(\mathbf{L}_*(\mathbf{x})-\mathbf{L}_c)(\mathbf{g}_t-t\mathbf{g}_1)=-\frac{1}{t}\mathbf{F}\cdot\mathbf{X}(t)\mathbf{F}.$$

By (3.25) we can rewrite (3.23) as

$$t\mathbf{F}\cdot\frac{d\mathbf{L}^e(t)}{dt}\mathbf{F}=-\fint_Y(\mathbf{g}_t-t\mathbf{g}_1)\cdot\mathbf{L}_c(\mathbf{g}_t-t\mathbf{g}_1)+\mathbf{F}\cdot(t^2\mathbf{\Gamma}_2+2\mathbf{X}(t)+\mathbf{L}^e(t)-\mathbf{L}_c)\mathbf{F}.$$

Inserting $\frac{d\mathbf{L}^e(t)}{dt}=\frac{d\mathbf{X}(t)}{dt}+\mathbf{\Gamma}_1+2t\mathbf{\Gamma}_2$ into the above equation, we obtain

$$\mathbf{F}\cdot[t\frac{d\mathbf{X}(t)}{dt}-3\mathbf{X}(t)]\mathbf{F}=-\fint_Y(\mathbf{g}_t-t\mathbf{g}_1)\cdot\mathbf{L}_c(\mathbf{g}_t-t\mathbf{g}_1)\qquad\forall\,t\in(0,1). \tag{3.26}$$

The above differential identity has profound implication in the behavior of the flow $t\mapsto\mathbf{L}^e(t)$, as will be shown shortly.

3.3 Proof of the upper bound

Below we find a lower bound for the integral $\fint_Y (\mathbf{g}_t - t\mathbf{g}_1) \cdot \mathbf{L}_c(\mathbf{g}_t - t\mathbf{g}_1)$ which is the negative of the right hand side of (3.26). By Lemma 1, (2.6), we have that for any nonzero $\mathbf{E} \in \mathbb{U}$,

$$\fint_Y (\mathbf{g}_t - t\mathbf{g}_1) \cdot \mathbf{L}_c(\mathbf{g}_t - t\mathbf{g}_1) \geq \rho_{\mathbf{g}}(\mathbf{L}_c, \mathbf{E}) \fint_Y |\mathbf{E} \cdot (\mathbf{g}_t - t\mathbf{g}_1)|^2. \tag{3.27}$$

Subsequently, we write $\rho_{\mathbf{g}}(\mathbf{L}_c, \mathbf{E})$ briefly as $\rho_{\mathbf{g}}$ when there is no danger of confusion. By the Jensen's inequality we bound the right hand side of (3.27) from below as

$$\fint_Y |\mathbf{E} \cdot (\mathbf{g}_t - t\mathbf{g}_1)|^2 \geq \sum_{\alpha=0}^{N} \theta_\alpha \Big[\fint_{\Omega_\alpha} \mathbf{E} \cdot (\mathbf{g}_t - t\mathbf{g}_1)\Big]^2 = \sum_{\alpha=0}^{N} \theta_\alpha |\mathbf{E} \cdot \mathbf{F}_\alpha|^2. \tag{3.28}$$

where

$$\mathbf{F}_\alpha = \fint_{\Omega_\alpha} (\mathbf{g}_t - t\mathbf{g}_1) \qquad (\alpha = 0, \cdots, N). \tag{3.29}$$

Since $\fint_Y (\mathbf{g}_t - t\mathbf{g}_1) = 0$, by (3.29) and (3.16) we have

$$\sum_{\alpha=0}^{N} \theta_\alpha \mathbf{F}_\alpha = 0, \qquad \sum_{\alpha=0}^{N} \theta_\alpha \mathbf{L}_\alpha \mathbf{F}_\alpha = \frac{1}{t}\mathbf{X}(t)\mathbf{F}. \tag{3.30}$$

Therefore, the right hand side of (3.28) is bounded from below by

$$\min\Big\{\sum_{\alpha=0}^{N} \theta_\alpha |\mathbf{E} \cdot \mathbf{F}_\alpha|^2 : \ \mathbf{F}_\alpha \ (\alpha = 0, \cdots, N) \text{ satisfy } (3.30)\Big\} =: Q(\frac{1}{t}\mathbf{X}(t)\mathbf{F}). \tag{3.31}$$

It is straightforward to verify that the above minimum $Q(\frac{1}{t}\mathbf{X}(t)\mathbf{F})$ is nonnegative and depends on its argument quadratically. [1] Therefore, we can identify a positive semi-definite tensor $\mathbf{C} : \mathbb{U} \to \mathbb{U}$, independent of t, such that

$$Q(\frac{1}{t}\mathbf{X}(t)\mathbf{F}) = \frac{1}{t^2}\mathbf{F} \cdot \mathbf{X}(t)\mathbf{C}\mathbf{X}(t)\mathbf{F}. \tag{3.32}$$

In summary, by (3.27), (3.28), (3.31) and (3.32) we conclude that

$$\fint_Y (\mathbf{g}_t - t\mathbf{g}_1) \cdot \mathbf{L}_c(\mathbf{g}_t - t\mathbf{g}_1) \geq \frac{\rho_{\mathbf{g}}}{t^2}\mathbf{F} \cdot \mathbf{X}(t)\mathbf{C}\mathbf{X}(t)\mathbf{F}. \tag{3.33}$$

By (3.33) and (3.26) we arrive at

$$t\frac{d\mathbf{X}(t)}{dt} - 3\mathbf{X}(t) + \frac{\rho_{\mathbf{g}}}{t^2}\mathbf{X}(t)\mathbf{C}\mathbf{X}(t) \leq 0 \qquad \forall\, t \in (0, 1). \tag{3.34}$$

[1] The minimization problem (3.31) can be rewritten as a standard quadratic programming problem: $\min\{\mathbf{x} \cdot \mathbf{A}\mathbf{x} : \mathbf{B}\mathbf{x} = \mathbf{c}\}$, where the components of the $p \times 1$ vector $\mathbf{x}$ are those of the matrix $\mathbf{F}_\alpha$, the components of the $q \times 1$ vector $\mathbf{c}$ are either zero or the components of $\mathbf{X}(t)\mathbf{F}/t$, and the $p \times p$ matrix $\mathbf{A}$ and $q \times p$ matrix $\mathbf{B}$, independent of t, are such that $\mathbf{x} \cdot \mathbf{A}\mathbf{x}$ is equal to $\sum_{\alpha=0}^{N} \frac{1}{|\Omega_\alpha|}|\mathbf{E} \cdot \mathbf{F}_\alpha|^2$ and $\mathbf{B}\mathbf{x} = \mathbf{c}$ is equivalent to the constraints in (3.30). By the method of Lagrangian multiplier, we formally find the minimum of this quadratic programming problem is given by $\mathbf{c} \cdot (\mathbf{B}\mathbf{A}^{-1}\mathbf{B}^T)^{-1}\mathbf{c}$, which is a quadratic function of $\mathbf{c}$ and hence a quadratic function of $\mathbf{X}(t)\mathbf{F}/t$.

Let $\mathbf{X}(t) = \tilde{\mathbf{X}}(t)t^3$. Then equation (3.34) implies that

$$\begin{cases} \frac{d\tilde{\mathbf{X}}(t)}{dt} + \rho_{\mathbf{g}}\tilde{\mathbf{X}}(t)\mathbf{C}\tilde{\mathbf{X}}(t) \le 0 & \forall\, t \in (0,1), \\ \tilde{\mathbf{X}}(t) = \mathbf{\Gamma}_3 & \text{if } t = 0. \end{cases} \tag{3.35}$$

Assume that the tensor

$$\tilde{\mathbf{X}}_0(t) = \Big(\mathbf{\Gamma}_3^{-1} + t\rho_{\mathbf{g}}\mathbf{C}\Big)^{-1} = \mathbf{\Gamma}_3\Big(\mathbb{I} + t\rho_{\mathbf{g}}\mathbf{C}\mathbf{\Gamma}_3\Big)^{-1} \tag{3.36}$$

is non-singular for $t \in [0,1]$. Then direct calculations reveal that $\tilde{\mathbf{X}}_0(t)$ satisfies that

$$\begin{cases} \frac{d\tilde{\mathbf{X}}_0(t)}{dt} + \rho_{\mathbf{g}}\tilde{\mathbf{X}}_0(t)\mathbf{C}\tilde{\mathbf{X}}_0(t) = 0 & \text{if } t \in (0,1), \\ \tilde{\mathbf{X}}_0(t) = \mathbf{\Gamma}_3 & \text{if } t = 0. \end{cases} \tag{3.37}$$

Setting $\tilde{\mathbf{X}}_1(t) = \tilde{\mathbf{X}}_0(t) - \tilde{\mathbf{X}}(t)$, by (3.35) and (3.37) we obtain

$$\begin{cases} \frac{d\tilde{\mathbf{X}}_1(t)}{dt} + \tilde{\mathbf{X}}_1(t)\mathbf{B} + \mathbf{B}^T\tilde{\mathbf{X}}_1(t) + \rho_{\mathbf{g}}\tilde{\mathbf{X}}_1(t)\mathbf{C}\tilde{\mathbf{X}}_1(t) =: \mathbf{Z}(t) \ge 0 & \text{if } t \in (0,1), \\ \tilde{\mathbf{X}}_1(t) = 0 & \text{if } t = 0. \end{cases} \tag{3.38}$$

where $\mathbf{B} = \rho_{\mathbf{g}}\mathbf{C}\tilde{\mathbf{X}}(t)$. We recognize that the above equations are *Riccati differential equations*, see Reid (1972) [42]. An application of the comparison theorem [42, 14] will yield restrictions on the trajectories of $t \mapsto \mathbf{X}_1(t)$ and hence $t \mapsto \mathbf{L}^e(t)$ which can be interpreted as cross-property relations. In particular, if the behavior of $\mathbf{L}^e(t)$ is known as $t \to 0$, then the restrictions imply bounds on the final values of $\mathbf{L}^e(1)$, i.e., the interested effective tensor $\mathbf{L}^e_*$.

For the reader's convenience, we outline below the argument of the comparison theorem. The Riccati differential equations $(3.38)_1$ are closely related with the linear differential system for $\mathcal{U}, \mathcal{V} : [0,1] \to \mathbb{L}$,

$$\begin{cases} -\mathcal{V}'(t) + \mathbf{Z}(t)\mathcal{U}(t) - \mathbf{B}^T(t)\mathcal{V}(t) = 0, \\ \mathcal{U}'(t) - \mathbf{B}(t)\mathcal{U}(t) - \rho_{\mathbf{g}}\mathbf{C}\mathcal{V}(t) = 0. \end{cases} \tag{3.39}$$

Let $0 \le t_1 < t_2 \le 1$, and denote by $\mathcal{U}_{t_1}, \mathcal{V}_{t_1} : [t_1, t_2] \to \mathbb{L}$ the solutions to (3.39) with initial conditions

$$\mathcal{U}(t_1) = \mathbb{I}, \qquad \mathcal{V}(t_1) = \tilde{\mathbf{X}}_1(t_1). \tag{3.40}$$

Further, for any given nonzero $\mathbf{F} \in \mathbb{U}$ we denote by

$$\mathbf{U}(t) = \mathcal{U}_{t_1}(t)\mathbf{F}, \qquad \mathbf{V}(t) = \mathcal{V}_{t_1}(t)\mathbf{F}.$$

It is clear from (3.39)-(3.40) that $\mathbf{U}, \mathbf{V} : [t_1, t_2] \to \mathbb{U}$ satisfy that

$$\tilde{\mathbf{X}}_1(t_1)\mathbf{U}(t_1) - \mathbf{V}(t_1) = \tilde{\mathbf{X}}_1(t_1)\mathbf{F} - \tilde{\mathbf{X}}_1(t_1)\mathbf{F} = 0, \tag{3.41}$$

and that

$$\begin{cases} -\mathbf{V}'(t) + \mathbf{Z}(t)\mathbf{U}(t) - \mathbf{B}^T\mathbf{V}(t) = 0, \\ \mathbf{U}'(t) - \mathbf{B}\mathbf{U}(t) - \rho_{\mathbf{g}}\mathbf{C}\mathbf{V}(t) = 0. \end{cases} \tag{3.42}$$

From the above equation it is easy to check that

$$\frac{d}{dt}[\mathbf{U}(t)\cdot\mathbf{V}(t)] = \rho_{\mathbf{g}}\mathbf{V}(t)\cdot\mathbf{C}\mathbf{V}(t) + \mathbf{U}(t)\cdot\mathbf{Z}(t)\mathbf{U}(t). \tag{3.43}$$

Let

$$J = \mathbf{U}(t_1)\cdot\tilde{\mathbf{X}}_1(t_1)\mathbf{U}(t_1) + \int_{t_1}^{t_2}\Big\{\rho_{\mathbf{g}}\mathbf{V}(t)\cdot\mathbf{C}\mathbf{V}(t) + \mathbf{U}(t)\cdot\mathbf{Z}(t)\mathbf{U}(t)\Big\}dt. \tag{3.44}$$

By (3.43) and (3.41) we have

$$J = \mathbf{U}(t_1)\cdot[\tilde{\mathbf{X}}_1(t_1)\mathbf{U}(t_1) - \mathbf{V}(t_1)] + \mathbf{U}(t_2)\cdot\mathbf{V}(t_2) = \mathbf{U}(t_2)\cdot\mathbf{V}(t_2). \tag{3.45}$$

If $\tilde{\mathbf{X}}_1(t_1) > 0$, equation (3.44) implies $J > 0$ for any nonzero $\mathbf{F}\in\mathbb{U}$ and hence, by (3.45), $\mathcal{U}_{t_1}(t)$ and $\mathcal{V}_{t_1}(t)$ are nonsingular for any $t\in[t_1,t_2]$. Consequently, $\mathcal{V}_{t_1}(t)\mathcal{U}_{t_1}^{-1}(t)$ is well-defined and we can easily verify that it satisfies (3.38). By the uniqueness of the solution to (3.38) with initial conditions at $t = t_1$, we conclude that

$$\tilde{\mathbf{X}}_1(t) = \mathcal{V}_{t_1}(t)\mathcal{U}_{t_1}^{-1}(t) \in \mathbb{L}^+_{\text{sym}} \qquad \forall\, t\in[t_1,t_2].$$

Further, if we have merely $\tilde{\mathbf{X}}_1(t_1) \geq 0$, for $\varepsilon > 0$ let $\tilde{\mathbf{X}}_{1\varepsilon} = \tilde{\mathbf{X}}_1(t_1) + \varepsilon\mathbf{I\!I}$ and denote by $\tilde{\mathbf{X}}_1^\varepsilon(t)$ the solution to $(3.38)_1$ satisfying $\tilde{\mathbf{X}}_1^\varepsilon(t_1) = \tilde{\mathbf{X}}_{1\varepsilon}$. By the result just established the solution $\tilde{\mathbf{X}}_1^\varepsilon(t)$ exists on $[t_1,t_2]$ and $\tilde{\mathbf{X}}_1^\varepsilon(t) > 0$ on $[t_1,t_2]$. Further, Theorem 4.1 of [42] implies that $\tilde{\mathbf{X}}_1^\varepsilon(t)\to\tilde{\mathbf{X}}_1(t)$ as $\varepsilon\to 0$, and henceforth $\tilde{\mathbf{X}}_1(t)\geq 0$ on $[t_1,t_2]$. In conclusion, by $(3.38)_2$ we have

$$\tilde{\mathbf{X}}_1(t) \geq 0 \quad \forall\, t\in[0,1]. \tag{3.46}$$

We summarize below.

Theorem 3 *Let $\mathbf{L}_c\in\mathbb{L}^+_{\text{ellip}}$ be a comparison tensor, $\mathbf{L}(\mathbf{x},t)\in\mathbb{L}^+_{\text{ellip}}$ for $t\in[0,1]$ such that the effective tensor $\mathbf{L}^e(t)$ is well-defined by (3.5) and (3.7), $\mathbf{\Gamma}_i$ be the coefficient tensors of the expansion (3.13), $\mathbf{E}\in\mathbb{U}$ be a nonzero matrix, $\rho_{\mathbf{g}} = \rho_{\mathbf{g}}(\mathbf{L}_c,\mathbf{E}) > 0$ be given by (2.2), and $\mathbf{C}\geq 0$ be given by (3.31) and (3.32).*

(i) (**Bound**) *The effective tensor $\mathbf{L}^e(t)$ satisfies (3.46), i.e.,*

$$\mathbf{L}^e(t) - \mathbf{\Gamma}_0 - t\mathbf{\Gamma}_1 - t^2\mathbf{\Gamma}_2 \leq t^3(\mathbf{\Gamma}_3^{-1} + t\rho_{\mathbf{g}}\mathbf{C})^{-1} \quad \forall\, t\in[0,1]. \tag{3.47}$$

(ii) (**Attainment condition**) *Equality holds for (3.47) if and only if the solution $\mathbf{g}_t\in\mathbb{G}$ to the inhomogeneous Eshelby inclusion problem (3.6) and the solution $\mathbf{g}_1$ to the homogeneous Eshelby inclusion problem $(3.10)_1$ satisfy that for some $c_{\mathbf{k}}\in\mathbb{C}$ and $p_\alpha\in\mathbb{R}$,*

$$\begin{cases}\mathbf{g}_t - t\mathbf{g}_1 = \sum_{\mathbf{k}\in\mathcal{K}\cap\mathcal{S}_{\mathbf{g}}(\mathbf{L},\mathbf{E})}\hat{\mathbf{u}}_{\mathbf{k}}\otimes\hat{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{x}), & \hat{\mathbf{u}}_{\mathbf{k}} = c_{\mathbf{k}}\mathbf{N}\mathbf{E}\hat{\mathbf{k}}.\\ \mathbf{E}\cdot(\mathbf{g}_t - t\mathbf{g}_1) = \sum_{\alpha=0}^{N} p_\alpha\chi_\alpha\end{cases} \qquad \forall\, t\in[0,1].$$

4 Bounds on the effective compliance tensors

We remark that the exposition of this section is parallel to the last section and the relevant calculations proceed likewise. This is not completely obvious; appropriate notations are essential for uncovering this similarity and the corresponding quantities have different physical meanings.

4.1 Series expansions of the divergence-free fields and effective compliant tensors

For the inhomogeneous medium (3.1) and an average applied stress $\mathbf{P} \in \mathbb{U}$, we can alternately formulate the problem (3.2) as follows: find $\boldsymbol{\sigma}_* \in \mathbb{P}$ such that

$$\mathbf{M}_*(\mathbf{x})(\boldsymbol{\sigma}_* + \mathbf{P}) \in \mathbb{G} \oplus \mathbb{U}, \tag{4.1}$$

where

$$\mathbf{M}_*(\mathbf{x}) = [\mathbf{L}_*(\mathbf{x})]^{-1} = \mathbf{L}_\alpha^{-1} \qquad \text{if } \mathbf{x} \in \Omega_\alpha, \ \alpha = 0, \cdots, N.$$

Let $\mathbf{M}_c = \mathbf{L}_c^{-1}$,

$$\mathbf{M}(\mathbf{x}, t) = \mathbf{M}_c + t(\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c) \in \mathbb{L}^+_{\text{sym}} \tag{4.2}$$

be the compliance tensor interpolating between the homogeneous comparison medium $\mathbf{M}_c$ and the inhomogeneous medium $\mathbf{M}_*(\mathbf{x})$ when t varies in $[0, 1]$. For any $\mathbf{P} \in \mathbb{U}$, define

$$\mathcal{E}^d(\mathbf{P}, t) = \mathbf{P} \cdot \mathbf{M}^e(t)\mathbf{P} = \min_{\boldsymbol{\sigma} \in \mathbb{P}} \fint_Y [(\boldsymbol{\sigma} + \mathbf{P}) \cdot \mathbf{M}(\mathbf{x}, t)(\boldsymbol{\sigma} + \mathbf{P})]. \tag{4.3}$$

The associated Euler-Lagrangian equation implies that the minimizer $\boldsymbol{\sigma}_t \in \mathbb{P}$ satisfies

$$\mathbf{M}(\mathbf{x}, t)(\boldsymbol{\sigma}_t + \mathbf{P}) \in \mathbb{G} \oplus \mathbb{U}. \tag{4.4}$$

Clearly, if $t = 0$, the medium is homogeneous, and the solution to (4.4) satisfies $\boldsymbol{\sigma}_t = 0$ and $\mathcal{E}^d(\mathbf{P}, 0) = 0$. Assume a small perturbation, i.e., $0 < t << 1$. It can be shown that the solutions to (4.4) can be written as

$$\boldsymbol{\sigma}_t = t\boldsymbol{\sigma}_1 + t^2\boldsymbol{\sigma}_2 + t^3\boldsymbol{\sigma}_3 + \cdots . \tag{4.5}$$

Inserting the above expression into (4.4) and arranging terms according to the order of t, we find

$$[\mathbf{M}_c + t(\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)](\mathbf{P} + t\boldsymbol{\sigma}_1 + t^2\boldsymbol{\sigma}_2 + t^3\boldsymbol{\sigma}_3 + \cdots) \in \mathbb{G} \oplus \mathbb{U}, \tag{4.6}$$

which implies that $\boldsymbol{\sigma}_i \in \mathbb{P}$ $(i = 1, 2, \cdots)$ necessarily satisfy

$$\begin{cases} \mathbf{M}_c\boldsymbol{\sigma}_1 + (\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)\mathbf{P} \in \mathbb{G} \oplus \mathbb{U} & \text{if } i = 1, \\ \mathbf{M}_c\boldsymbol{\sigma}_i + (\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)\boldsymbol{\sigma}_{i-1} \in \mathbb{G} \oplus \mathbb{U} & \text{if } i > 1. \end{cases} \tag{4.7}$$

Let $\mathbf{F} = \fint_Y (\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)\mathbf{P}$ and $\tilde{\mathbf{g}}_1 \in \mathbb{G}$ be such that

$$\tilde{\mathbf{g}}_1 + \mathbf{F} = \mathbf{M}_c\boldsymbol{\sigma}_1 + (\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)\mathbf{P}. \tag{4.8}$$

Operating $\mathbf{L}_c$ on both sides of the above equation yields

$$\mathbf{L}_c\tilde{\mathbf{g}}_1 - \mathbf{L}_c\mathbf{M}_*(\mathbf{x})\mathbf{P} \in \mathbb{P} \oplus \mathbb{U}, \tag{4.9}$$

which can be identified as a homogeneous Eshelby inclusion problem (5.2) with eigenstress $-\mathbf{L}_c\mathbf{M}_\alpha\mathbf{P}$ on Ω_α $(\alpha = 0, \cdots, N)$. By (4.3) and (4.5) we have the following expansion:

$$\mathbf{M}^e(t) = \sum_{i=0}^{\infty} t^i\boldsymbol{\Lambda}_i = \boldsymbol{\Lambda}_0 + t\boldsymbol{\Lambda}_1 + t^2\boldsymbol{\Lambda}_2 + t^3\boldsymbol{\Lambda}_3 + o(t^3). \tag{4.10}$$

To find the expansion coefficient tensors $\mathbf{\Lambda}_i$, we differentiate (4.3) with respect to $\mathbf{P}$ and, by (4.3), (4.6) and (4.10), obtain

$$2\sum_{i=0}^{\infty} t^i \mathbf{\Lambda}_i \mathbf{P} = 2\mathbf{M}_c\mathbf{F} + 2t\Big[\fint_Y \mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c\Big]\mathbf{P} + 2t\fint_Y (\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)\boldsymbol{\sigma}_t.$$

Therefore,

$$\mathbf{\Lambda}_0 = \mathbf{M}_c, \qquad \mathbf{\Lambda}_1 = -\mathbf{M}_c + \fint_Y \mathbf{M}_*(\mathbf{x}), \tag{4.11}$$

and

$$\mathbf{\Lambda}_{i+1}\mathbf{P} = \fint_Y (\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)\boldsymbol{\sigma}_i \qquad \text{if } i = 1, 2, \cdots . \tag{4.12}$$

Also, we have

$$(\mathbf{M}^e(t) - \mathbf{\Lambda}_0 - t\mathbf{\Lambda}_1 - t^2\mathbf{\Lambda}_2)\mathbf{P} = \sum_{i=3}^{\infty} t^i \mathbf{\Lambda}_i \mathbf{P} = t\fint_Y (\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)(\boldsymbol{\sigma}_t - t\boldsymbol{\sigma}_1). \tag{4.13}$$

and the following theorem.

Theorem 4 *For any integer $i \geq 1$, let $\mathbf{\Lambda}_i$ be the expansion coefficient tensors satisfying (4.10) and $\boldsymbol{\sigma}_i \in \mathbb{G}$ satisfy (4.7). Then,*

$$\begin{aligned} &\fint_Y \boldsymbol{\sigma}_i \cdot \mathbf{M}_c \boldsymbol{\sigma}_j = -\mathbf{P} \cdot \mathbf{\Lambda}_{i+j}\mathbf{P}, \\ &\fint_Y \boldsymbol{\sigma}_i \cdot (\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)\boldsymbol{\sigma}_j = \mathbf{P} \cdot \mathbf{\Lambda}_{i+j+1}\mathbf{P}, \end{aligned} \tag{4.14}$$

Again, we note that the above theorem implies that

$$\begin{aligned} \mathbf{P} \cdot \mathbf{\Lambda}_{2i}\mathbf{P} &= -\fint_Y \boldsymbol{\sigma}_i \cdot \mathbf{M}_c \boldsymbol{\sigma}_i, \\ \mathbf{P} \cdot \mathbf{\Lambda}_{2i+1}\mathbf{P} &= \fint_Y \boldsymbol{\sigma}_i \cdot (\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)\boldsymbol{\sigma}_i, \end{aligned} \tag{4.15}$$

meaning that to determine the coefficient tensors $\mathbf{\Lambda}_0, \cdots, \mathbf{\Lambda}_{2i+1}$, it is sufficient to solve (4.7) for $\boldsymbol{\sigma}_1, \cdots, \boldsymbol{\sigma}_i$. The proof of the above Theorem is similar to that of Theorem 2 and will not be repeated here.

4.2 A dual differential identity

Parallel to Section 3.2, we derive a differential identity for the effective compliant tensor $\mathbf{M}^e(t)$ in this section. Differentiating (4.3) with respect to t, we obtain

$$\mathbf{P} \cdot \frac{d\mathbf{M}^e(t)}{dt}\mathbf{P} = \fint_Y (\boldsymbol{\sigma}_t + \mathbf{P}) \cdot (\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)(\boldsymbol{\sigma}_t + \mathbf{P}). \tag{4.16}$$

By (4.2) we rewrite the right hand side of the above equation as

$$\begin{aligned} &\fint_Y \Big\{\frac{1}{t}(\boldsymbol{\sigma}_t + \mathbf{P}) \cdot \mathbf{M}(\mathbf{x}, t)(\boldsymbol{\sigma}_t + \mathbf{P}) - \frac{1}{t}(\boldsymbol{\sigma}_t + \mathbf{P}) \cdot \mathbf{M}_c(\boldsymbol{\sigma}_t + \mathbf{P})\Big\} \\ &\quad = \frac{1}{t}\Big[-\fint_Y \boldsymbol{\sigma}_t \cdot \mathbf{M}_c \boldsymbol{\sigma}_t + \mathbf{P} \cdot (\mathbf{M}^e(t) - \mathbf{M}_c)\mathbf{P}\Big], \end{aligned}$$

which implies the following identity

$$t\mathbf{P}\cdot\frac{d\mathbf{M}^e(t)}{dt}\mathbf{P}=-\!\!\!\!\!\!\int_Y\boldsymbol{\sigma}_t\cdot\mathbf{M}_c\boldsymbol{\sigma}_t+\mathbf{P}\cdot(\mathbf{M}^e(t)-\mathbf{M}_c)\mathbf{P}\qquad\forall\,t\in(0,1).\tag{4.17}$$

Let

$$\mathbf{Y}(t)=\mathbf{M}^e(t)-\boldsymbol{\Lambda}_0-t\boldsymbol{\Lambda}_1-t^2\boldsymbol{\Lambda}_2.\tag{4.18}$$

Then

$$\begin{aligned}-\!\!\!\!\!\!\int_Y\boldsymbol{\sigma}_t\cdot\mathbf{M}_c\boldsymbol{\sigma}_t&=-\!\!\!\!\!\!\int_Y(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1+t\boldsymbol{\sigma}_1)\cdot\mathbf{M}_c(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1+t\boldsymbol{\sigma}_1)\\&=-\!\!\!\!\!\!\int_Y[t^2\boldsymbol{\sigma}_1\cdot\mathbf{M}_c\boldsymbol{\sigma}_1+2t\boldsymbol{\sigma}_1\cdot\mathbf{L}_c(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)+(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)\cdot\mathbf{M}_c(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)]\\&=-t^2\mathbf{P}\cdot\boldsymbol{\Lambda}_2\mathbf{P}-2\mathbf{P}\cdot\mathbf{Y}(t)\mathbf{P}+-\!\!\!\!\!\!\int_Y(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)\cdot\mathbf{M}_c(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)\end{aligned}\tag{4.19}$$

where for the last equality we have used $(4.15)_1$ with $i=1$ and, by (1.6), $(4.7)_1$, (4.12) and (4.13), the identity

$$-\!\!\!\!\!\!\int_Y\boldsymbol{\sigma}_1\cdot\mathbf{M}_c(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)=-\mathbf{P}\cdot-\!\!\!\!\!\!\int_Y(\mathbf{M}_*(\mathbf{x})-\mathbf{L}_c)(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)=-\frac{1}{t}\mathbf{P}\cdot\mathbf{Y}(t)\mathbf{P}.$$

By (3.23) and (3.25) we can rewrite (4.17) as

$$t\mathbf{P}\cdot\frac{d\mathbf{M}^e(t)}{dt}\mathbf{P}=-\!\!\!\!\!\!\int_Y(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)\cdot\mathbf{M}_c(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)+\mathbf{P}\cdot(t^2\boldsymbol{\Lambda}_2+2\mathbf{Y}(t)+\mathbf{M}^e(t)-\mathbf{M}_c)\mathbf{P}.$$

Inserting $\frac{d\mathbf{M}^e(t)}{dt}=\frac{d\mathbf{Y}(t)}{dt}+\boldsymbol{\Lambda}_1+2t\boldsymbol{\Lambda}_2$ into the above equation, we obtain

$$\mathbf{P}\cdot[t\frac{d\mathbf{Y}(t)}{dt}-3\mathbf{Y}(t)]\mathbf{P}=-\!\!\!\!\!\!\int_Y(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)\cdot\mathbf{M}_c(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)\qquad\forall\,t\in(0,1).\tag{4.20}$$

The above differential equality has profound implications in the behavior of the flow $t\mapsto\mathbf{M}^e(t)$, as will be shown shortly.

4.3 Proof of the dual (lower) bound

As in Section 3.3, below we derive a differential inequality for $\mathbf{M}^e(t)$. We first focus on the first term on the right hand side of (4.20). Applying Lemma 1, (2.8) to $\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1$, we have that for any nonzero $\mathbf{E}\in\mathbb{U}$,

$$-\!\!\!\!\!\!\int_Y(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)\cdot\mathbf{M}_c(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)\geq\rho_{\boldsymbol{\sigma}}(\mathbf{L}_c,\mathbf{E})-\!\!\!\!\!\!\int_Y|\mathbf{E}\cdot(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)|^2.\tag{4.21}$$

Subsequently, for brevity we write $\rho_{\boldsymbol{\sigma}}(\mathbf{L}_c,\mathbf{E})$ briefly as $\rho_{\boldsymbol{\sigma}}$ when there is no danger of confusion. By the Jensen's inequality we bound the right hand side of (4.21) from below as

$$-\!\!\!\!\!\!\int_Y|\mathbf{E}\cdot(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)|^2\geq\sum_{\alpha=0}^N\theta_\alpha\Big[-\!\!\!\!\!\!\int_{\Omega_\alpha}\mathbf{E}\cdot(\boldsymbol{\sigma}_t-t\boldsymbol{\sigma}_1)\Big]^2=\sum_{\alpha=0}^N\theta_\alpha|\mathbf{E}\cdot\mathbf{P}_\alpha|^2.\tag{4.22}$$

where $|\Omega_\alpha|$ denotes the volume of the domain Ω_α,

$$\mathbf{P}_\alpha = \fint_{\Omega_\alpha} (\boldsymbol{\sigma}_t - t\boldsymbol{\sigma}_1) \qquad (\alpha = 0, \cdots, N). \tag{4.23}$$

Since $\boldsymbol{\sigma}_t,\ \boldsymbol{\sigma}_1 \in \mathbb{P}$, by (4.23) and (4.13) we have

$$\sum_{\alpha=0}^{N} \theta_\alpha \mathbf{P}_\alpha = 0, \qquad \sum_{\alpha=0}^{N} \theta_\alpha \mathbf{M}_\alpha \mathbf{P}_\alpha = \frac{1}{t}\mathbf{Y}(t)\mathbf{P}. \tag{4.24}$$

Therefore, to bound from below the right hand side of (4.22) we consider the algebraic minimization problem

$$\min\Big\{\sum_{\alpha=0}^{N} \frac{1}{|\Omega_\alpha|}|\mathbf{E}\cdot\mathbf{P}_\alpha|^2 :\ \mathbf{F}_\alpha\ (\alpha = 0, \cdots, N) \text{ satisfy } (4.24)\Big\} =: Q^d(\frac{1}{t}\mathbf{Y}(t)\mathbf{P}). \tag{4.25}$$

As before, we can verify that the above minimum $Q^d(\frac{1}{t}\mathbf{Y}(t)\mathbf{P})$ is nonnegative and depends on its argument quadratically, see footnote on page 12. Therefore, we can identify a nonnegative tensor $\mathbf{D} \in \overline{\mathbb{L}^+_{sym}}$, independent of t, such that

$$Q^d(\frac{1}{t}\mathbf{Y}(t)\mathbf{P}) = \frac{1}{t^2}\mathbf{P}\cdot\mathbf{Y}(t)\mathbf{D}\mathbf{Y}(t)\mathbf{P}. \tag{4.26}$$

By (4.21), (4.22), (4.25) and (4.26) we conclude that

$$\fint_{Y} (\boldsymbol{\sigma}_t - t\boldsymbol{\sigma}_1)\cdot\mathbf{M}_c(\boldsymbol{\sigma}_t - t\boldsymbol{\sigma}_1) \geq \frac{\rho_{\boldsymbol{\sigma}}}{t^2}\mathbf{P}\cdot\mathbf{Y}(t)\mathbf{D}\mathbf{Y}(t)\mathbf{P}. \tag{4.27}$$

By (4.20) and (4.27) we arrive at

$$t\frac{d\mathbf{Y}(t)}{dt} + \frac{\rho_{\boldsymbol{\sigma}}}{t^2}\mathbf{Y}(t)\mathbf{D}\mathbf{Y}(t) - 3\mathbf{Y}(t) \leq 0 \qquad \forall\, t \in (0,1). \tag{4.28}$$

Let $\mathbf{Y}(t) = \tilde{\mathbf{Y}}(t)t^3$. Then equation (4.28) implies that

$$\frac{d\tilde{\mathbf{Y}}(t)}{dt} + \rho_{\boldsymbol{\sigma}}\tilde{\mathbf{Y}}(t)\mathbf{D}\tilde{\mathbf{Y}}(t) \leq 0 \qquad \forall\, t \in (0,1). \tag{4.29}$$

Assume that the tensor

$$\tilde{\mathbf{Y}}_0(t) = \Big(\boldsymbol{\Lambda}_3^{-1} + t\rho_{\boldsymbol{\sigma}}\mathbf{D}\Big)^{-1} = \boldsymbol{\Lambda}_3\Big(\mathbf{I\!I} + t\rho_{\boldsymbol{\sigma}}\mathbf{D}\boldsymbol{\Lambda}_3\Big)^{-1} \tag{4.30}$$

is well-defined for $t \in [0,1]$. Then direct calculations reveal that $\tilde{\mathbf{Y}}_0(t)$ satisfies that

$$\begin{cases} \frac{d\tilde{\mathbf{Y}}_0(t)}{dt} + \rho_{\boldsymbol{\sigma}}\tilde{\mathbf{Y}}_0(t)\mathbf{D}\tilde{\mathbf{Y}}_0(t) = 0 & \text{if } t \in (0,1), \\ \tilde{\mathbf{Y}}_0(t) = \boldsymbol{\Lambda}_3 & \text{if } t = 0. \end{cases} \tag{4.31}$$

Setting $\tilde{\mathbf{Y}}_1(t) = \tilde{\mathbf{Y}}_0(t) - \tilde{\mathbf{Y}}(t)$, by (4.29) and (4.31) we obtain

$$\begin{cases} \frac{d\tilde{\mathbf{Y}}_1(t)}{dt} + \tilde{\mathbf{Y}}_1(t)\mathbf{B}' + \mathbf{B}'^T\tilde{\mathbf{Y}}_1(t) + \rho_{\boldsymbol{\sigma}}\tilde{\mathbf{Y}}_1(t)\mathbf{D}\tilde{\mathbf{Y}}_1(t) \geq 0 & \text{if } t \in (0,1), \\ \tilde{\mathbf{Y}}_1(t) = 0 & \text{if } t = 0. \end{cases} \tag{4.32}$$

where $\mathbf{B}' = \rho_{\boldsymbol{\sigma}}\mathbf{D}\tilde{\mathbf{Y}}(t)$. We notice that the above equations are the same *Riccati differential equations* as in (4.32). Similar argument as for Theorem 3 implies that

$$\tilde{\mathbf{Y}}_1(t) \geq 0 \quad \text{if } t \in [0,1]. \tag{4.33}$$

We summarize below.

Theorem 5 *Let $\mathbf{L}_c \in \mathbb{L}^+_{\text{ellip}}$ be a comparison tensor, $\mathbf{M}(\mathbf{x},t) \geq 0$ for $t \in [0,1]$ such that the effective tensor $\mathbf{M}^e(t)$ is well-defined by (4.3), $\mathbf{\Lambda}_i$ be the coefficient tensors in the expansion (4.10), $\mathbf{E} \in \mathbb{U}$ be a nonzero matrix, $\rho_{\boldsymbol{\sigma}} = \rho_{\boldsymbol{\sigma}}(\mathbf{L}_c, \mathbf{E}) > 0$ be given by (2.3), and $\mathbf{D} \in \overline{\mathbb{L}^+_{sym}}$ be given by (4.25) and (4.26).*

(i) (**Bound**) *The effective tensor $\mathbf{M}^e(t)$ satisfies (4.33), i.e.,*

$$\mathbf{M}^e(t) - \mathbf{\Lambda}_0 - t\mathbf{\Lambda}_1 - t^2\mathbf{\Lambda}_2 \leq t^3(\mathbf{\Lambda}_3^{-1} + t\rho_{\boldsymbol{\sigma}}\mathbf{D})^{-1} \qquad \forall\, t \in [0,1]. \tag{4.34}$$

(ii) (**Attainment condition**) *Equality holds for (4.34) if and only if the solution $\boldsymbol{\sigma}_t \in \mathbb{P}$ to the inhomogeneous Eshelby inclusion problem (4.4) and the solution $\boldsymbol{\sigma}_1 \in \mathbb{P}$ to the homogeneous Eshelby inclusion problem $(4.7)_1$ satisfy that for some $c_{\mathbf{k}} \in \mathbb{C}$ and $p_\alpha \in \mathbb{R}$,*

$$\begin{cases} \boldsymbol{\sigma}_t - t\boldsymbol{\sigma}_1 = \sum_{\mathbf{k}\in\mathcal{K}\cap\mathcal{S}_{\boldsymbol{\sigma}}(\mathbf{L},\mathbf{E})} \hat{\boldsymbol{\sigma}}_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{x}), \qquad \hat{\boldsymbol{\sigma}}_{\mathbf{k}} = c_{\mathbf{k}}[\mathbf{L}\mathbf{E} - \mathbf{L}(\mathbf{N}\boldsymbol{\omega}) \otimes \hat{\mathbf{k}}]. \\ \mathbf{E}\cdot(\boldsymbol{\sigma}_t - t\boldsymbol{\sigma}_1) = \sum_{\alpha=0}^N p_\alpha \chi_\alpha \end{cases} \quad \forall\, t \in [0,1].$$

5 Explicit bounds in terms of average Eshelby tensors

As mentioned before, the average Eshelby tensors are important for the analysis based on the Eshelby's solutions, in the Mori-Tanaka's theory, and the models in account of the surface and interface effects. In our approach, the average Eshelby tensors for the homogeneous problem provide initial conditions as $t \to 0$ for the applications of the comparison theorem. The resulting energy bounds therefore depend on the microstructure through the average Eshelby tensors and a residual term. The residual term can often be bounded from below or above by algebraic conditions of the media, but its exact evaluation requires knowledge of the actual field on the inclusion. To obtain the microstructure-independent bounds, we may further perform a maximization problem over all possible average Eshelby tensors. Therefore, a characterization of all possible average Eshelby tensors is important for the quality of the obtained microstructure-independent bounds. Further, the characterization of the set of average Eshelby tensors is also useful for classifying microstructues and the solutions to inverse problems.

5.1 Average Eshelby tensors

Below we obtain the Fourier representation of the average Eshelby tensors for the classic and periodic Eshelby inclusion problems. Restrictions on the Eshelby tensors follow from this representation. We remark that due to its applications, particularly in the framework of Mori-Tanaka theory, the classic homogeneous Eshelby inclusion problems in $\mathbb{R}^n$ have been addressed by many authors in a variety of situations. The periodic Eshelby inclusion problems in two dimensions are addressed in Liu (2010). Also, the reader is cautioned that our formulation of the Eshelby inclusion problem and definition of the average Eshelby tensor are slightly different from the usual convention; we use eigenstress instead of eigenstrain as the source term. Certain properties including the symmetry and positive-definiteness of the Eshelby tensors are more transparent in this convention.

Let $\mathbf{P}_\alpha \in \mathbb{U}$ ($\alpha = 0, \cdots, N$) be the eigenstress on the αth-phase. For a piecewise-constant eigenstress

$$\mathbf{P}_* = \sum_{\alpha=0}^N \mathbf{P}_\alpha \chi_\alpha, \tag{5.1}$$

and homogeneous comparison medium $\mathbf{L}_c \in \mathbb{L}^+_{\text{ellip}}$, the periodic *homogeneous* Eshelby inclusion problem is to find $\mathbf{g} \in \mathbb{G}$ such that

$$\mathbf{L}_c\mathbf{g} + \mathbf{P}_* \in \mathbb{P} \oplus \mathbb{U}. \tag{5.2}$$

In Fourier space, the above equation implies that

$$\hat{\mathbf{g}}(\mathbf{k}) = -\sum_{\alpha=0}^{N} [\mathbf{N}(\mathbf{P}_\alpha \hat{\mathbf{k}})] \otimes \hat{\mathbf{k}} \hat{\chi}_\alpha(\mathbf{k}),$$

where we recall $\hat{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$ and $\mathbf{N}$ is the inverse matrix of $(\mathbf{L})_{piqj}(\hat{\mathbf{k}})_i(\hat{\mathbf{k}})_j$. Therefore, by the Parseval's theorem we have

$$\theta_\alpha \bar{\mathbf{g}}_\alpha := \fint_Y \chi_\alpha \mathbf{g} = -\sum_{\mathbf{k}\in\mathcal{K}} \sum_{\beta=0}^{N} [\mathbf{N}\mathbf{P}_\beta \hat{\mathbf{k}}] \otimes \hat{\mathbf{k}} \hat{\chi}^{\text{conj}}_\alpha(\mathbf{k}) \hat{\chi}_\beta(\mathbf{k}). \tag{5.3}$$

The above equation can be rewritten as

$$\fint_Y \chi_\alpha \mathbf{g} = -\sum_{\beta=0}^{N} \mathbf{T}^{\alpha\beta} \mathbf{P}_\beta, \tag{5.4}$$

where $\mathbf{T}^{\alpha\beta}$ is given by

$$(\mathbf{T}^{\alpha\beta})_{piqj} = \sum_{\mathbf{k}\in\mathcal{K}} (\mathbf{N})_{pq} (\hat{\mathbf{k}})_i (\hat{\mathbf{k}})_j \hat{\chi}^{\text{conj}}_\alpha(\mathbf{k}) \hat{\chi}_\beta(\mathbf{k}) \tag{5.5}$$

and can be recognized as the average Eshelby tensor.

From the representation (5.5), we immediately obtain the following properties of the linear mapping $\mathbf{T}^{\alpha\beta} : \mathbb{U} \to \mathbb{U}$:

(i) $\mathbf{T}^{\alpha\beta} = (\mathbf{T}^{\alpha\beta})^{\text{conj}} = \mathbf{T}^{\beta\alpha} \qquad \forall\, \alpha,\ \beta = 0, \cdots, N;$

(ii) $(\mathbf{T}^{\alpha\beta})_{piqj} = (\mathbf{T}^{\alpha\beta})_{qjpi} \qquad \forall\, \alpha,\ \beta = 0, \cdots, N;$

(iii) $\sum_{\beta=0}^{N} \mathbf{T}^{\alpha\beta} = 0 \qquad \forall\, \alpha = 0, \cdots, N;$

(iv) $\sum_{\alpha,\beta=0}^{N} \mathbf{P}^\alpha \cdot \mathbf{T}^{\alpha\beta} \mathbf{P}^\beta = \fint_Y \mathbf{g} \cdot \mathbf{L}_c \mathbf{g} \geq 0 \qquad \forall\, \mathbf{P}^\alpha \in \mathbb{U}\ (\alpha = 0, \cdots, N);$

In addition, we notice that

$$\sum_{\mathbf{k}\in\mathcal{K}} \hat{\chi}^{\text{conj}}_\alpha(\mathbf{k}) \hat{\chi}_\beta(\mathbf{k}) = \fint_Y (\chi_\alpha - \theta_\alpha)(\chi_\beta - \theta_\beta) = \begin{cases} \theta_\alpha(1-\theta_\alpha) & \text{if } \alpha = \beta, \\ -\theta_\alpha \theta_\beta & \text{if } \alpha \neq \beta. \end{cases}$$

5.2 Upper bound

We now relate the coefficient tensors $\boldsymbol{\Gamma}_i$ $(i = 2, 3)$ with the average Eshelby tensors $\mathbf{T}^{\alpha\beta}$ defined above. From (3.15) and (5.4), we have

$$\boldsymbol{\Gamma}_2 = -\sum_{\alpha,\beta=0}^{N} \triangle\mathbf{L}_\alpha \mathbf{T}^{\alpha\beta} \triangle\mathbf{L}_\beta. \tag{5.6}$$

Let

$$\gamma = \fint_Y \Big(\mathbf{g}_1 - \sum_{\alpha=0}^N \bar{\mathbf{g}}_\alpha \chi_\alpha\Big) \cdot (\mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c)\Big(\mathbf{g}_1 - \sum_{\alpha=0}^N \bar{\mathbf{g}}_\alpha \chi_\alpha\Big),$$
$$\mathbf{\Gamma}_{3B} = \sum_{\alpha=0}^N \sum_{\beta'=0}^N \sum_{\beta=0}^N \frac{\theta_\alpha}{\theta_\beta \theta_{\beta'}} \triangle \mathbf{L}_{\beta'} \mathbf{T}^{\alpha\beta'} \triangle \mathbf{L}_\alpha \mathbf{T}^{\alpha\beta} \triangle \mathbf{L}_\beta. \tag{5.7}$$

Then by (3.18) and (5.3) we have

$$\begin{aligned}\mathbf{F} \cdot \mathbf{\Gamma}_3 \mathbf{F} &= \fint_Y \Big(\mathbf{g}_1 - \sum_{\alpha=0}^N \bar{\mathbf{g}}_\alpha \chi_\alpha + \sum_{\alpha=0}^N \bar{\mathbf{g}}_\alpha \chi_\alpha\Big) \cdot (\mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c)\Big(\mathbf{g}_1 - \sum_{\alpha=0}^N \bar{\mathbf{g}}_\alpha \chi_\alpha + \sum_{\alpha=0}^N \bar{\mathbf{g}}_\alpha \chi_\alpha\Big) \\ &= \gamma + \fint_Y \Big(\sum_{\alpha=0}^N \bar{\mathbf{g}}_\alpha \chi_\alpha\Big) \cdot (\mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c)\Big(\sum_{\alpha=0}^N \bar{\mathbf{g}}_\alpha \chi_\alpha\Big) \\ &= \gamma + \mathbf{F} \cdot \mathbf{\Gamma}_{3B} \mathbf{F},\end{aligned} \tag{5.8}$$

where the last equality follows from (5.3)-(5.7). If $\mathbf{L}_*(\mathbf{x}) - \mathbf{L}_c \le 0$, it is clear that $\gamma \le 0$ and $\mathbf{\Gamma}_3 \le \mathbf{\Gamma}_{3B}$. Therefore, the bound (3.46) can be rewritten as

$$\mathbf{L}^e(t) - \mathbf{\Gamma}_0 - t\mathbf{\Gamma}_1 - t^2 \mathbf{\Gamma}_2 \le t^3 (\mathbf{\Gamma}_{3B}^{-1} + t\rho_{\mathbf{g}} \mathbf{C})^{-1} \quad \forall\, t \in [0, 1]. \tag{5.9}$$

From (3.14), (5.6) and (5.7) we see that the above upper bound explicitly depends on the average Eshelby tensors of the microstructure. If we have a good estimate or precise calculation of the average Eshelby tensors, the above bound is presumably much better than the microstructure-indpendent bound, especially for high-contrast composites.

5.3 Dual bound — lower bound

Similarly, We can relate the coefficient tensors $\mathbf{\Lambda}_i$ $(i = 2, 3)$ with the average Eshelby tensors $\mathbf{T}^{\alpha\beta}$. By (4.9) we have that ($\overline{\mathbf{M}} = \fint_Y \mathbf{M}_*(\mathbf{x})$)

$$\boldsymbol{\sigma}_1 = \mathbf{L}_c \tilde{\mathbf{g}}_1 + \mathbf{L}_c\big(\overline{\mathbf{M}} - \mathbf{M}_*(\mathbf{x})\big)\mathbf{P},$$

and hence, by (5.3)-(5.4), obtain

$$\theta_\alpha \bar{\boldsymbol{\sigma}}_\alpha := \fint_Y \boldsymbol{\sigma}_1 \chi_\alpha \quad = \mathbf{L}_c \Big(\textstyle\sum_{\beta=0}^N \mathbf{T}^{\alpha\beta} \mathbf{L}_c \triangle \mathbf{M}_\beta \mathbf{P} + \theta_\alpha (\overline{\mathbf{M}} - \mathbf{M}_\alpha)\mathbf{P}\Big). \tag{5.10}$$

Therefore, by (4.12) we find that

$$\begin{aligned}\mathbf{\Lambda}_2 \mathbf{P} &= \fint_Y (\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)\boldsymbol{\sigma}_1 = \sum_{\alpha=0}^N \triangle \mathbf{M}_\alpha \fint_Y \boldsymbol{\sigma}_1 \chi_\alpha \\ &= \sum_{\alpha=0}^N \Big[\triangle \mathbf{M}_\alpha \mathbf{L}_c \sum_{\beta=0}^N \mathbf{T}^{\alpha\beta} \mathbf{L}_c \triangle \mathbf{M}_\beta + \theta_\alpha \triangle \mathbf{M}_\alpha \mathbf{L}_c (\overline{\mathbf{M}} - \mathbf{M}_\alpha)\Big]\mathbf{P}.\end{aligned}$$

That is,

$$\mathbf{\Lambda}_2 = \sum_{\alpha=0}^N \sum_{\beta=0}^N \triangle \mathbf{M}_\alpha \mathbf{L}_c \mathbf{T}^{\alpha\beta} \mathbf{L}_c \triangle \mathbf{M}_\beta + \sum_{\alpha=0}^N \theta_\alpha (\overline{\mathbf{M}} - \triangle \mathbf{M}_\alpha) \mathbf{L}_c (\overline{\mathbf{M}} - \mathbf{M}_\alpha). \tag{5.11}$$

Further, let

$$\gamma^d = \fint_Y \Big(\boldsymbol{\sigma}_1 - \sum_{\alpha=0}^N \bar{\boldsymbol{\sigma}}_\alpha \chi_\alpha\Big) \cdot (\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)\Big(\boldsymbol{\sigma}_1 - \sum_{\alpha=0}^N \bar{\boldsymbol{\sigma}}_\alpha \chi_\alpha\Big),$$

$$\begin{aligned}\boldsymbol{\Lambda}_{3B} = &\sum_{\alpha,\beta,\beta'=0}^N \frac{\theta_\alpha}{\theta_\beta \theta_{\beta'}} \triangle\mathbf{M}_{\beta'}\mathbf{L}_c\mathbf{T}^{\alpha\beta'}\mathbf{L}_c\triangle\mathbf{M}_\alpha\mathbf{L}_c\mathbf{T}^{\alpha\beta}\mathbf{L}_c\triangle\mathbf{M}_\beta \\ &+ 2\sum_{\alpha,\beta'=0}^N \frac{\theta_\alpha}{\theta_{\beta'}} \triangle\mathbf{M}_{\beta'}\mathbf{L}_c\mathbf{T}^{\alpha\beta'}\mathbf{L}_c\triangle\mathbf{M}_\alpha\mathbf{L}_c(\overline{\mathbf{M}} - \mathbf{M}_\alpha) + \sum_{\alpha=0}^N \theta_\alpha(\overline{\mathbf{M}} - \mathbf{M}_\alpha)\mathbf{L}_c\triangle\mathbf{M}_\alpha\mathbf{L}_c(\overline{\mathbf{M}} - \mathbf{M}_\alpha).\end{aligned} \tag{5.12}$$

Then, by (4.15) we have

$$\begin{aligned}\mathbf{P}\cdot\boldsymbol{\Lambda}_3\mathbf{P} &= \fint_Y \Big(\boldsymbol{\sigma}_1 - \sum_{\alpha=0}^N \bar{\boldsymbol{\sigma}}_\alpha\chi_\alpha + \sum_{\alpha=0}^N \bar{\boldsymbol{\sigma}}_\alpha\chi_\alpha\Big) \cdot (\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)\Big(\boldsymbol{\sigma}_1 - \sum_{\alpha=0}^N \bar{\boldsymbol{\sigma}}_\alpha\chi_\alpha + \sum_{\alpha=0}^N \bar{\boldsymbol{\sigma}}_\alpha\chi_\alpha\Big) \\ &= \gamma^d + \fint_Y \Big(\sum_{\alpha=0}^N \bar{\boldsymbol{\sigma}}_\alpha\chi_\alpha\Big)\cdot(\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c)\Big(\sum_{\alpha=0}^N \bar{\boldsymbol{\sigma}}_\alpha\chi_\alpha\Big) = \gamma^d + \mathbf{P}\cdot\boldsymbol{\Lambda}_{3B}\mathbf{P},\end{aligned} \tag{5.13}$$

If $\mathbf{M}_*(\mathbf{x}) - \mathbf{M}_c \le 0$, it is clear that $\gamma^d \le 0$ and $\boldsymbol{\Lambda}_3 \le \boldsymbol{\Lambda}_{3B}$. Therefore, the bound (4.34) can be rewritten as

$$\mathbf{M}^e(t) - \boldsymbol{\Lambda}_0 - t\boldsymbol{\Lambda}_1 - t^2\boldsymbol{\Lambda}_2 \le t^3(\boldsymbol{\Lambda}_{3B}^{-1} + t\rho_{\boldsymbol{\sigma}}\mathbf{D})^{-1} \qquad \forall\, t\in[0,1]. \tag{5.14}$$

From (4.11), (5.11) and (5.12) we see that the above dual bound (i.e., lower bound for $\mathbf{L}^e(t)$) explicitly depends on the average Eshelby tensors of the microstructure. If we have a good estimate or precise calculation of the average Eshelby tensors, the above bound is much better than the microstructure-indpendent bound, especially for high-contrast composites.

6 Summary and Discussion

In this paper we present a differential approach to microstructure-dependent bounds for multiphase composites. Based on the perturbation method, we derive a differential inequality satisfied by the effective tensors with the initial condition determined by solving the homogeneous Eshelby inclusion problem. The relevant differential equations are a Riccati differential system. An application of comparison theorem yields the desired microstructure-dependent bounds in terms of the average Eshelby tensors. Since the average Eshelby tensors is much easier to exactly compute or reasonably estimate based on micrographs of the microstructures of the composites, the microstructure-dependent bounds are unsurprisingly much tighter than the microstructure-independent Hashin-Shtrikman's bounds.

Although the final explicit bounds (5.9) and (5.14) in terms of the average Eshelby tensors still require the usual condition of well-orderedness, the bounds (3.47) and (4.34) are valid for any comparison tensor $\mathbf{L}_c$. With this additional degree of freedom, we anticipate the bounds (3.47) and (4.34) are useful in estimating effective properties of non-well-ordered composites such as polycrystals and improving bounds for multiphase composites where it is known that the Hashin-Shtrikamn bounds are no longer optimal [26].

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