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Universal bounds for effective piezoelectric moduli

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Abstract

Rigorous upper and lower bounds for the effective moduli are obtained for heterogeneous piezoelectric materials, by generalizing the Hashin–Shtrikman variational principle to the coupled problems of piezoelectricity. The key in obtaining these bounds is the choice of the field variables used in the variational principles, i.e., the strain tensor and the electric displacement vector or the stress tensor and the electric field vector. Universal theorems, originally established for (uncoupled) mechanical and non-mechanical problems, are generalized for application to piezoelectricity problems, and the boundary conditions which provide upper and lower bounds for the average energy are identified. These theorems lead to rigorous bounds for the effective piezoelectric moduli that are defined through the relation between the average field quantities. Computable bounds are derived from Eshelby's tensors for the piezoelectricity problems. These tensors are obtained by applying the Fourier transform to the Green's functions of an unbounded homogeneous body.

1. Introduction

Micromechanics has been used to predict the effective properties of heterogeneous materials, particularly, to obtain upper and lower bounds for the overall properties of composites. The estimate of such bounds were initiated in pioneering works by Hashin and Shtrikman (1962), and later by Walpole (1966), Kröner (1977), and Willis (1977); see more recent works by Francfort and Murat (1986), Milton and Kohn (1988), Milton (1990), and Torquato (1991, 1992); see also Nemat-Nasser and Hori (1993, 1995), Balendran and Nemat-Nasser (1995), and Munashinghe et al. (1996). Essentially the same procedure has been applied to predict bounds for both (uncoupled) mechanical and non-mechanical properties, such as effective moduli, and electric, magnetic, or diffusive properties. However, much less attention has been paid to the coupled mechanical and non-mechanical properties; see, for instance, Dunn and Taya (1994) and Benveniste (1997).

In this paper, we consider the case of piezoelectricity as an illustrative example of predicting bounds for coupled mechanical and non-mechanical properties. The formulation presented here can be applied to other cases of coupled problems. The field variables are: the displacement, strain, and stress, $(\boldsymbol{u}, \boldsymbol{\epsilon}, \boldsymbol{\sigma})$, for the mechanical behavior; and the electric potential, electric field, and electric displacement, $(u, \boldsymbol{p}, \boldsymbol{q})$, for the non-mechanical response.

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Symbolic notation is mainly used in this paper; a vector or tensor quantity is denoted by a bold face letter. The first-, and second-order contractions, and the tensor product are denoted by $\cdot$ and :, and $\otimes$, respectively, and ∇ stands for the spatial derivative; for instance, $\nabla \cdot \boldsymbol{\sigma}$ and $\nabla \otimes \boldsymbol{u}$ correspond to $\partial\sigma_{ij}/\partial x_i$ and $\partial u_j/\partial x_i$ in index notation.

2. Summary of piezoelectric field equations

We summarize three sets of field equations which govern the spatial variation of the field variables, $(\boldsymbol{u}, \boldsymbol{\epsilon}, \boldsymbol{\sigma})$ and $(u, \boldsymbol{p}, \boldsymbol{q})$. The first set ensures mechanical equilibrium and the absence of free charge,

$$\nabla \cdot \boldsymbol{\sigma}(\boldsymbol{x}) = 0, \qquad \nabla \cdot \boldsymbol{q}(\boldsymbol{x}) = 0. \tag{1}$$

The second set defines the strain tensor, $\boldsymbol{\epsilon}$, and the electric field, $\boldsymbol{p}$, in terms of the displacement vector, $\boldsymbol{u}$, and the electric potential, u,

$$\boldsymbol{\epsilon}(\boldsymbol{x}) = \frac{1}{2}(\nabla \otimes \boldsymbol{u}(\boldsymbol{x}) + (\nabla \otimes \boldsymbol{u}(\boldsymbol{x}))^{\mathrm{T}}), \qquad \boldsymbol{p}(\boldsymbol{x}) = -\nabla u(\boldsymbol{x}). \tag{2}$$

The third set is constitutive, relating the strain and electric field, $\boldsymbol{\epsilon}$ and $\boldsymbol{p}$, to the stress and electric displacement, $\boldsymbol{\sigma}$ and $\boldsymbol{q}$; for coupled [1] mechanical and electric problems, the following linear relations relate $\boldsymbol{\epsilon}$ and $\boldsymbol{q}$ to $\boldsymbol{\sigma}$ and $\boldsymbol{p}$:

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{C}(\boldsymbol{x}) : \boldsymbol{\epsilon}(\boldsymbol{x}) + \boldsymbol{H}(\boldsymbol{x}) \cdot \boldsymbol{q}(\boldsymbol{x}), \qquad \boldsymbol{p}(\boldsymbol{x}) = \boldsymbol{H}^{\mathrm{T}}(\boldsymbol{x}) : \boldsymbol{\epsilon}(\boldsymbol{x}) + \boldsymbol{R}(\boldsymbol{x}) \cdot \boldsymbol{q}(\boldsymbol{x}). \tag{3}$$

where [2] $\boldsymbol{C}$, $\boldsymbol{H}$, and $\boldsymbol{R}$ are fourth-, third-, and second-order tensors, satisfying the following symmetry properties: $C_{ijkl} = C_{jikl} = C_{ijlk}$, $H_{ijk} = H_{jik}$, and $R_{ij} = R_{ji}$. The inverse relations corresponding to Eq. (3) are

$$\boldsymbol{\epsilon}(\boldsymbol{x}) = \boldsymbol{D}(\boldsymbol{x}) : \boldsymbol{\sigma}(\boldsymbol{x}) + \boldsymbol{L}(\boldsymbol{x}) \cdot \boldsymbol{p}(\boldsymbol{x}), \qquad \boldsymbol{q}(\boldsymbol{x}) = \boldsymbol{L}^{\mathrm{T}}(\boldsymbol{x}) : \boldsymbol{\sigma}(\boldsymbol{x}) + \boldsymbol{K}(\boldsymbol{x}) \cdot \boldsymbol{p}(\boldsymbol{x}),$$

where $\boldsymbol{D} = (\boldsymbol{C} - \boldsymbol{H} \cdot \boldsymbol{K}' \cdot \boldsymbol{H}^{\mathrm{T}})^{-1}$, $\boldsymbol{K} = (\boldsymbol{R} - \boldsymbol{H}^{\mathrm{T}} : \boldsymbol{C}^{-1} : \boldsymbol{H})^{-1}$, and $\boldsymbol{L} = -(\boldsymbol{C}')^{-1} : \boldsymbol{H} \cdot \boldsymbol{K}'$.

Coupled governing equations for the mechanical displacement, $\boldsymbol{u}$, and the electric potential, u, can be derived from the three sets of the field equations, Eqs. (1)–(3). To obtain the governing equations, we rewrite the constitutive relations (3), which relate $(\boldsymbol{\epsilon}, \boldsymbol{q})$ and $(\boldsymbol{\sigma}, \boldsymbol{p})$, in an alternative form which relates $(\boldsymbol{\epsilon}, \boldsymbol{p})$ and $(\boldsymbol{\sigma}, \boldsymbol{q})$, i.e.,

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{C}'(\boldsymbol{x}) : \boldsymbol{\epsilon}(\boldsymbol{x}) + \boldsymbol{L}'(\boldsymbol{x}) \cdot \boldsymbol{p}(\boldsymbol{x}), \qquad \boldsymbol{q}(\boldsymbol{x}) = -(\boldsymbol{L}'(\boldsymbol{x}))^{\mathrm{T}} : \boldsymbol{\epsilon}(\boldsymbol{x}) + \boldsymbol{K}'(\boldsymbol{x}) \cdot \boldsymbol{p}(\boldsymbol{x}), \tag{4}$$

where $\boldsymbol{C}' = \boldsymbol{D}^{-1}$, $\boldsymbol{K}' = \boldsymbol{R}^{-1}$, and $\boldsymbol{L}' = \boldsymbol{H} \cdot \boldsymbol{K}'$. Then, substituting Eqs. (2) and (4) into Eq. (1), we obtain the governing equations as follows:

$$\begin{aligned} &\nabla \cdot (\boldsymbol{C}'(\boldsymbol{x}) : (\nabla \otimes \boldsymbol{u}(\boldsymbol{x}))) - \nabla \cdot (\boldsymbol{L}'(\boldsymbol{x}) \cdot (\nabla u(\boldsymbol{x}))) = 0, \\ &-\nabla \cdot ((\boldsymbol{L}'(\boldsymbol{x}))^{\mathrm{T}} : (\nabla \otimes \boldsymbol{u}(\boldsymbol{x}))) - \nabla \cdot (\boldsymbol{K}'(\boldsymbol{x}) \cdot (\nabla u(\boldsymbol{x}))) = 0; \end{aligned} \tag{5}$$

see Fig. 1 for a schematic view of the three sets of the field equations for the statical and kinematical quantities. To simplify expressions, we will omit the argument $\boldsymbol{x}$ of the field variables in the following sections.

[1] Constitutive relations (3) were originally proposed by Lothe and Barnett (1977); see also Lothe and Barnett (1976). In this form, the coupling moduli retain a certain symmetry, i.e., $H_{ijk}q_k$ and $H_{ijk}\epsilon_{ij}$ occur in the expressions for σ_{ij} and p_k, respectively. This is in contrast to the representation (4) which uses anti-symmetric coupling moduli, i.e., $L'_{ijk}p_k$ and $-L'_{ijk}\epsilon_{ij}$ occur in the expressions for σ_{ij} and q_k.

[2] Superscript T on a third-order tensor stands for *transpose* in a symbolic sense so that $\boldsymbol{H}^{\mathrm{T}} : \boldsymbol{\epsilon}$ corresponds to $H_{kli}\epsilon_{kl}$.

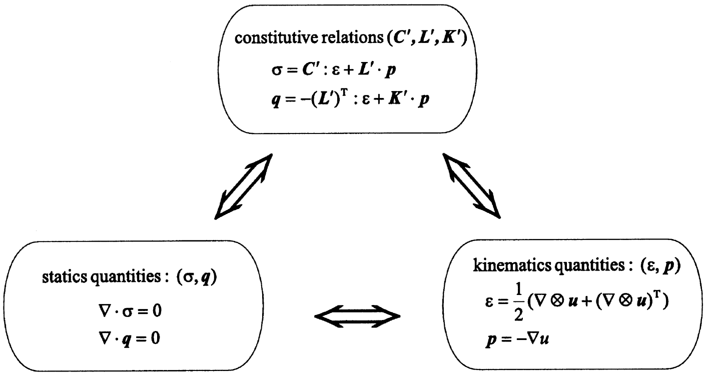

Fig. 1. Field equations of piezoelectricity.

3. Averaging and universal theorems

In this section, the averaging and two universal theorems, originally established for uncoupled mechanical or non-mechanical problems (Nemat-Nasser and Hori, 1993), are generalized and applied to the coupled problems. The two universal theorems play a key role in computing bounds for the coupled effective piezoelectric moduli.

3.1. Averaging theorems

Averaging theorems give the volume average of a field variable in terms of the corresponding surface data. There are three sets of the averaging theorems for uncoupled mechanical and non-mechanical problems, namely, the averaging theorem for the kinematical quantities ($\boldsymbol{\epsilon}$ and $\boldsymbol{p}$), the statical (or dynamical) quantities ($\boldsymbol{\sigma}$ and $\boldsymbol{q}$), and their products which relate to the energy ($\boldsymbol{\sigma} : \boldsymbol{\epsilon}$ and $\boldsymbol{q} \cdot \boldsymbol{p}$). These averaging theorems are applied to a material of arbitrary constitutive properties (linear or non-linear), since they are derived from Eqs. (1) and (2). Thus, they hold for the coupled problems.

We first present the averaging theorems for the kinematical and statical quantities, introducing a *representative volume element* (RVE) of volume V bounded by ∂V. The surface data, whether prescribed or not, are denoted by a superscript 0 on the corresponding quantity, e.g., $\boldsymbol{u}^0$, $\boldsymbol{t}^0$, u^0, and q^0, respectively, stand for surface [3] displacements, tractions, electric potential, and electric flux. The volume average of the associated field variable, taken over the RVE, is then given in terms of the surface data as follows:

$$\langle \boldsymbol{\epsilon} \rangle = \frac{1}{2V} \int_{\partial V} (\boldsymbol{v} \otimes \boldsymbol{u}^0 + \boldsymbol{u}^0 \otimes \boldsymbol{v} \, \mathrm{d}S), \qquad \langle \boldsymbol{\sigma} \rangle = \frac{1}{V} \int_{\partial V} \boldsymbol{x} \otimes \boldsymbol{t}^0 \, \mathrm{d}S,$$
$$\langle \boldsymbol{p} \rangle = -\frac{1}{V} \int_{\partial V} \boldsymbol{v} u^0 \, \mathrm{d}S, \qquad \langle \boldsymbol{q} \rangle = \frac{1}{V} \int_{\partial V} \boldsymbol{x} q^0 \, \mathrm{d}S, \tag{6}$$

where $\boldsymbol{v}$ is the (outer) unit normal vector on ∂V. The proof is straightforward: use [4] the Gauss theorem and the field equations, Eqs. (1) and (2).

[3] The tractions and electric flux satisfy $\boldsymbol{t}^0 = \boldsymbol{v} \cdot \boldsymbol{\sigma}$ and $q^0 = \boldsymbol{v} \cdot \mathbf{q}$ on ∂V.

[4] The four identities in Eq. (6) are all exact and valid independently of the constitutive properties. The same comments also apply to Eqs. (7) and (8).

The averaging theorems for the product of the strain and stress and the product of the electric field and electric displacement are also derived from Eqs. (1) and (2), as follows:

$$\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon} \rangle = \frac{1}{V} \int_{\partial V} \boldsymbol{t}^0 \cdot \boldsymbol{u}^0 \, \mathrm{d}S, \qquad \langle \boldsymbol{q} \cdot \boldsymbol{p} \rangle = -\frac{1}{V} \int_{\partial V} q^0 u^0 \, \mathrm{d}S. \tag{7}$$

Making use of the averaging theorems, Eqs. (6) and (7), we obtain the following identity which generalizes Hill's identity (Hill, 1963) to the coupled problems:

$$(\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon} \rangle + \langle \boldsymbol{q} \cdot \boldsymbol{p} \rangle) - (\langle \boldsymbol{\sigma} \rangle : \langle \boldsymbol{\epsilon} \rangle + \langle \boldsymbol{q} \rangle \cdot \langle \boldsymbol{p} \rangle) = \frac{1}{V} \int_{\partial V} \big((\boldsymbol{u}^0 - \boldsymbol{x} \cdot \langle \boldsymbol{\epsilon} \rangle) \cdot (\boldsymbol{t}^0 - \boldsymbol{v} \cdot \langle \boldsymbol{\sigma} \rangle) + (u^0 - \boldsymbol{x} \cdot \langle \boldsymbol{p} \rangle)(q^0 - \boldsymbol{v} \cdot \langle \boldsymbol{q} \rangle) \big) \, \mathrm{d}S. \tag{8}$$

When the right side of Eq. (8) becomes negligibly small compared with $\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon} \rangle + \langle \boldsymbol{q} \cdot \boldsymbol{p} \rangle$ or $\langle \boldsymbol{\sigma} \rangle : \langle \boldsymbol{\epsilon} \rangle + \langle \boldsymbol{q} \rangle \cdot \langle \boldsymbol{p} \rangle$, we can assume that $\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon} \rangle + \langle \boldsymbol{q} \cdot \boldsymbol{p} \rangle$ is almost the same as $\langle \boldsymbol{\sigma} \rangle : \langle \boldsymbol{\epsilon} \rangle + \langle \boldsymbol{q} \rangle \cdot \langle \boldsymbol{p} \rangle$. Hence, the effective moduli relating $(\langle \boldsymbol{\epsilon} \rangle, \langle \boldsymbol{p} \rangle)$ to $(\langle \boldsymbol{\sigma} \rangle, \langle \boldsymbol{q} \rangle)$ yield the average coupled energy, $\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon} \rangle + \langle \boldsymbol{q} \cdot \boldsymbol{p} \rangle$. It is observed that the right side of Eq. (8) is negligibly small when V is *statistically homogeneous*; the proof is essentially the same as that for the case [5] of the uncoupled problems.

Instead of the statistical homogeneity, the equality $\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon} \rangle + \langle \boldsymbol{q} \cdot \boldsymbol{p} \rangle = \langle \boldsymbol{\sigma} \rangle : \langle \boldsymbol{\epsilon} \rangle + \langle \boldsymbol{q} \rangle \cdot \langle \boldsymbol{p} \rangle$ results when the boundary data are such that the right side of Eq. (8) vanishes. For instance, the following two boundary data are of this class:

$$(\boldsymbol{u}^0, q^0) = (\boldsymbol{x} \cdot \boldsymbol{E}, \boldsymbol{v} \cdot \boldsymbol{Q}), \tag{9}$$

and

$$(\boldsymbol{t}^0, u^0) = (\boldsymbol{v} \cdot \boldsymbol{\Sigma}, \boldsymbol{x} \cdot \boldsymbol{P}), \tag{10}$$

where $(\boldsymbol{E}, \boldsymbol{Q})$ and $(\boldsymbol{\Sigma}, \boldsymbol{P})$ are constants. It follows from Eq. (6) that Eqs. (9) and (10) lead to $(\langle \boldsymbol{\epsilon} \rangle, \langle \boldsymbol{q} \rangle) = (\boldsymbol{E}, \boldsymbol{Q})$ and $(\langle \boldsymbol{\sigma} \rangle, \langle \boldsymbol{p} \rangle) = (\boldsymbol{\Sigma}, \boldsymbol{P})$, respectively, as originally obtained by Hill (1963) for the uncoupled problems. The boundary data which make the right side of Eq. (8) zero will be referred to as the Hill-type.

3.2. Universal theorems

Examine general nonlinear cases when the material of a heterogeneous RVE admits [6] a potential function, ϕ, which depends on the strain tensor, $\boldsymbol{\epsilon}$, and the electric displacement, $\boldsymbol{q}$, such that the stress, $\boldsymbol{\sigma}$, and the electric field, $\boldsymbol{p}$, are given by

$$\boldsymbol{\sigma} = \frac{\partial \phi}{\partial \boldsymbol{\epsilon}}(\boldsymbol{x}; \boldsymbol{\epsilon}, \boldsymbol{q}), \qquad \boldsymbol{p} = \frac{\partial \phi}{\partial \boldsymbol{q}}(\boldsymbol{x}; \boldsymbol{\epsilon}, \boldsymbol{q}). \tag{11}$$

This includes both the linear and non-linear cases. Note that the potential ϕ is defined in terms of the strain $\boldsymbol{\epsilon}$ and the electric displacement $\boldsymbol{q}$, instead of the electric field $\boldsymbol{p}$.

Using the micropotential, ϕ, we define a macropotential, Φ, for V subject to the Hill-type boundary data, as follows:

[5] See, for instance, Nemat-Nasser and Hori (1993).

[6] It is not possible to express a suitable potential in terms of the strain $\boldsymbol{\epsilon}$ and the electric field $\boldsymbol{p}$, using the constitutive relations (4); the product of the stress and strain and the product of the electric field and displacement are given by $\boldsymbol{\epsilon} : (\boldsymbol{C}' : \boldsymbol{\epsilon} + \boldsymbol{L}' \cdot \boldsymbol{p})$ and $\boldsymbol{p} \cdot (-(\boldsymbol{L}')^{\mathrm{T}} : \boldsymbol{\epsilon} + \boldsymbol{K}' \cdot \boldsymbol{p})$, respectively, and the coupling terms in these expressions, $\boldsymbol{\epsilon} : \boldsymbol{L}' \cdot \boldsymbol{p}$ and $-\boldsymbol{p} \cdot (\boldsymbol{L}')^{\mathrm{T}} : \boldsymbol{\epsilon}$, vanish when these two products are summed.

$$\Phi(\boldsymbol{E},\boldsymbol{Q}) = \langle \phi(\boldsymbol{x};\boldsymbol{\epsilon}(\boldsymbol{x};\boldsymbol{E},\boldsymbol{Q}),\boldsymbol{q}(\boldsymbol{x};\boldsymbol{E},\boldsymbol{Q}))\rangle, \tag{12}$$

where $\boldsymbol{E}$ and $\boldsymbol{Q}$ are macrostrain and macro-electric displacement given by $(\boldsymbol{E},\boldsymbol{Q}) = (\langle\boldsymbol{\epsilon}\rangle,\langle\boldsymbol{q}\rangle)$, and $(\boldsymbol{\epsilon},\boldsymbol{q})$ are regarded as functions of $(\boldsymbol{E},\boldsymbol{Q})$. It is easily shown that this macropotential yields the corresponding macrostress and macro-electric field, $(\boldsymbol{\Sigma},\boldsymbol{P}) = (\langle\boldsymbol{\sigma}\rangle,\langle\boldsymbol{p}\rangle)$, as follows:

$$\boldsymbol{\Sigma} = \frac{\partial\Phi}{\partial\boldsymbol{E}}(\boldsymbol{E},\boldsymbol{Q}), \qquad \boldsymbol{P} = \frac{\partial\Phi}{\partial\boldsymbol{Q}}(\boldsymbol{E},\boldsymbol{Q}). \tag{13}$$

The proof is straightforward. It follows from the property of the Hill-type boundary data that the derivative of the right side of Eq. (12) with respect to $\boldsymbol{E}$ can be expressed as

$$\left\langle \frac{\partial\boldsymbol{\epsilon}}{\partial\boldsymbol{E}} : \boldsymbol{\sigma} + \frac{\partial\boldsymbol{q}}{\partial\boldsymbol{E}}\cdot\boldsymbol{p} \right\rangle = \left\langle \frac{\partial\boldsymbol{\epsilon}}{\partial\boldsymbol{E}} \right\rangle : \langle\boldsymbol{\sigma}\rangle + \left\langle \frac{\partial\boldsymbol{q}}{\partial\boldsymbol{E}} \right\rangle : \langle\boldsymbol{p}\rangle = \frac{\partial\langle\boldsymbol{\epsilon}\rangle}{\partial\boldsymbol{E}} : \langle\boldsymbol{\sigma}\rangle + \frac{\partial\langle\boldsymbol{q}\rangle}{\partial\boldsymbol{E}} : \langle\boldsymbol{p}\rangle.$$

By definition, we have

$$\frac{\partial\langle\boldsymbol{\epsilon}\rangle}{\partial\boldsymbol{E}} = \mathbf{1}^{(4s)}, \qquad \frac{\partial\langle\boldsymbol{q}\rangle}{\partial\boldsymbol{E}} = \mathbf{0},$$

where $\mathbf{1}^{(4s)}$ is the fourth-order (symmetric) identity tensor. Hence, Eq. $(13)_1$ is obtained. In a similar manner, we can verify Eq. $(13)_2$ using the derivative of Φ with respect to $\boldsymbol{Q}$.

For given constant $(\boldsymbol{E},\boldsymbol{Q})$, there are various Hill-type [7] boundary data satisfying $(\langle\boldsymbol{\epsilon}\rangle,\langle\boldsymbol{q}\rangle) = (\boldsymbol{E},\boldsymbol{Q})$. The macropotentials associated with these boundary data are not the same, unless the solid is statistically homogeneous. Hence, the value of the macropotential of a finite heterogeneous V varies depending on the boundary data. We examine this dependence of the macropotential on the boundary data.

Suppose that the micropotential ϕ is *convex*, i.e., for any two sets of the strain and the electric displacement, $(\boldsymbol{\epsilon}^{(\alpha)},\boldsymbol{q}^{(\alpha)})$ $(\alpha = 1,2)$, ϕ satisfies

$$\phi\big(\boldsymbol{\epsilon}^{(1)},\boldsymbol{q}^{(1)}\big) - \phi\big(\boldsymbol{\epsilon}^{(2)},\boldsymbol{q}^{(2)}\big) \geqslant \big(\boldsymbol{\epsilon}^{(1)} - \boldsymbol{\epsilon}^{(2)}\big):\frac{\partial\phi}{\partial\boldsymbol{\epsilon}}\big(\boldsymbol{\epsilon}^{(2)},\boldsymbol{q}^{(2)}\big) + \big(\boldsymbol{q}^{(1)} - \boldsymbol{q}^{(2)}\big)\cdot\frac{\partial\phi}{\partial\boldsymbol{q}}\big(\boldsymbol{\epsilon}^{(2)},\boldsymbol{q}^{(2)}\big), \tag{14}$$

where the equality holds only for $(\boldsymbol{\epsilon}^{(2)},\boldsymbol{q}^{(2)}) = (\boldsymbol{\epsilon}^{(1)},\boldsymbol{q}^{(1)})$. Let $(\boldsymbol{\epsilon}^{(1)},\boldsymbol{q}^{(1)}) = (\boldsymbol{\epsilon}^{G},\boldsymbol{q}^{G})$ be the strain and electric displacement fields due to *any* general boundary data, and $(\boldsymbol{\epsilon}^{(2)},\boldsymbol{q}^{(2)}) = (\boldsymbol{\epsilon}^{\Sigma P},\boldsymbol{q}^{\Sigma P})$ be those due to the uniform boundary data defined by Eq. (10), where superscripts G and ΣP emphasize that quantities are associated with general boundary data and the boundary data of Eq. (10), respectively.

Consider now all such general boundary data which produce the same overall average strain and electric displacement, i.e., let

$$\big(\langle\boldsymbol{\epsilon}^{G}\rangle,\langle\boldsymbol{q}^{G}\rangle\big) = \big(\langle\boldsymbol{\epsilon}^{\Sigma P}\rangle,\langle\boldsymbol{q}^{\Sigma P}\rangle\big) = (\boldsymbol{E},\boldsymbol{Q}).$$

It then follows from inequality (14) that

$$\Phi^{\Sigma P}(\boldsymbol{E},\boldsymbol{Q}) < \Phi^{G}(\boldsymbol{E},\boldsymbol{Q}). \tag{15}$$

Note that (15) is valid whether or not the general boundary data are of the Hill-type. To prove the inequality (15), take the volume average of (14) and obtain

[7] Note that when V is subjected to Hill-type boundary conditions, the macropotential can be defined as the volume average of the micropotential. Then, the inner product of $(\langle\boldsymbol{\epsilon}\rangle,\langle\boldsymbol{q}\rangle)$ and $(\langle\boldsymbol{\sigma}\rangle,\langle\boldsymbol{p}\rangle)$ equals $\langle\boldsymbol{\sigma} : \boldsymbol{\epsilon} + \boldsymbol{q}\cdot\boldsymbol{p}\rangle$, relating to energy.

Table 1
Micropotential and macropotential

Micropotential	$\phi(\boldsymbol{\epsilon},\boldsymbol{q})$	$\psi(\boldsymbol{\sigma},\boldsymbol{p})$
Gradient	$\boldsymbol{\sigma}=\frac{\partial\phi}{\partial\boldsymbol{\epsilon}}$	$\boldsymbol{\epsilon}=\frac{\partial\psi}{\partial\boldsymbol{\sigma}}$
	$\boldsymbol{p}=\frac{\partial\phi}{\partial\boldsymbol{q}}$	$\boldsymbol{q}=\frac{\partial\psi}{\partial\boldsymbol{p}}$
Macropotential	$\Phi(\boldsymbol{E},\boldsymbol{Q})$	$\Psi(\boldsymbol{\Sigma},\boldsymbol{P})$
Gradient	$\langle\boldsymbol{\sigma}\rangle=\frac{\partial\Phi}{\partial\boldsymbol{E}}$	$\langle\boldsymbol{\epsilon}\rangle=\frac{\partial\Psi}{\partial\boldsymbol{\Sigma}}$
	$\langle\boldsymbol{p}\rangle=\frac{\partial\Phi}{\partial\boldsymbol{Q}}$	$\langle\boldsymbol{q}\rangle=\frac{\partial\Psi}{\partial\boldsymbol{P}}$
Universal theorems	$\Phi^G>\Phi^{\Sigma P}$	$\Psi^G>\Psi^{EQ}$

$$\Phi^G(\boldsymbol{E},\boldsymbol{P})-\Phi^{\Sigma P}(\boldsymbol{E},\boldsymbol{P})>\frac{1}{V}\int_{\partial V}\left(\left(\boldsymbol{u}^G-\boldsymbol{u}^{\Sigma P}\right)\cdot(\boldsymbol{v}\cdot\boldsymbol{\Sigma})+\left(\boldsymbol{v}\cdot\left(\boldsymbol{q}^G-\ \boldsymbol{q}^{\Sigma P}\right)\right)(\boldsymbol{x}\cdot\boldsymbol{P})\right)\,\mathrm{d}S$$
$$=\left\langle\boldsymbol{\epsilon}^G-\boldsymbol{\epsilon}^{\Sigma P}\right\rangle:\boldsymbol{\Sigma}+\left\langle\boldsymbol{q}^G-\boldsymbol{q}^{\Sigma P}\right\rangle\cdot\boldsymbol{P},$$

where Eqs. (7) and (10) are used. From $\langle\boldsymbol{\epsilon}^G\rangle=\langle\boldsymbol{\epsilon}^{\Sigma P}\rangle$ and $\langle\boldsymbol{q}^G\rangle=\langle\boldsymbol{q}^{\Sigma P}\rangle$, inequality (15) is now obtained.

Similar results can be obtained if a micropotential [8], ψ, for $\boldsymbol{\sigma}$ and $\boldsymbol{p}$ is used. The corresponding macropotential is then defined for V by

$$\Psi(\boldsymbol{\Sigma},\boldsymbol{P})=\langle\psi(\boldsymbol{x};\boldsymbol{\sigma}(\boldsymbol{x};\boldsymbol{\Sigma},\boldsymbol{P}),\ \boldsymbol{p}(\boldsymbol{x};\boldsymbol{\Sigma},\boldsymbol{P}))\rangle, \tag{16}$$

where $\boldsymbol{\Sigma}$ and $\boldsymbol{P}$ are the corresponding macrostress and macro-electric field, given by $(\boldsymbol{\Sigma},\boldsymbol{P})=(\langle\boldsymbol{\sigma}\rangle,\langle\boldsymbol{p}\rangle)$. This macropotential has the following three properties (like Φ).

1. For the Hill-type boundary data, the macropotential yields the macrostrain and macro-electric displacement, as follows:

$$\boldsymbol{E}=\frac{\partial\Psi}{\partial\boldsymbol{\Sigma}}(\boldsymbol{\Sigma},\boldsymbol{P}),\qquad \boldsymbol{Q}=\frac{\partial\Psi}{\partial\boldsymbol{P}}(\boldsymbol{\Sigma},\boldsymbol{P}). \tag{17}$$

2. The value of the macropotential depends on the type of boundary data, even though these data produce the same macrostress and macro-electric field.
3. When the micropotential is convex, the macropotential satisfies

$$\Psi^{EQ}(\boldsymbol{\Sigma},\boldsymbol{P})<\Psi^G(\boldsymbol{\Sigma},\boldsymbol{P}), \tag{18}$$

where Ψ^G and Ψ^{EQ} are the macropotential for any general boundary data and for the uniform boundary data defined by Eq. (9), respectively.

Table 1 is a summary of the results which relate to the two macropotentials, Φ and Ψ. From inequalities (15) and (18) the following two universal theorems are now obtained:

Universal Theorem I. *For an RVE whose microconstituents admit a convex micropotential, $\phi(\boldsymbol{\epsilon},\boldsymbol{q})$, among all boundary data which produce the same average strain and electric displacement, $(\langle\boldsymbol{\epsilon}\rangle,\langle\boldsymbol{q}\rangle)=(\boldsymbol{E},\boldsymbol{Q})$, the boundary data of Eq. (10) associated with the uniform stress and electric field, render the total macropotential $\Phi(\boldsymbol{E},\boldsymbol{Q})$ an absolute minimum.*

[8] The micropotential ψ is related to ϕ through the following Legendre transform: $\psi+\phi=\boldsymbol{\sigma}:\boldsymbol{\epsilon}+\boldsymbol{q}\cdot\boldsymbol{p}$.

Universal Theorem II. *For an RVE whose microconstituents admit a convex micropotential, $\psi(\boldsymbol{\sigma}, \boldsymbol{p})$, among all boundary data which produce the same average stress and electric field, $(\langle\boldsymbol{\sigma}\rangle, \langle\boldsymbol{p}\rangle) = (\boldsymbol{\Sigma}, \boldsymbol{P})$, the boundary data of Eq. (9) associated with the uniform strain and electric displacement, render the total macropotential $\Psi(\boldsymbol{\Sigma}, \boldsymbol{P})$ an absolute minimum.*

It should be emphasized that Eqs. (13) and (17) with macroquantities defined as simple volume averages of the microquantities, hold only for the Hill-type boundary data, whereas inequalities (15) and (18) are valid for *any* general boundary data.

3.3. Application of universal theorems

When the material is linear, the micropotentials, ϕ and ψ, are expressed in terms of $(\boldsymbol{C}, \boldsymbol{H}, \boldsymbol{R})$ or $(\boldsymbol{D}, \boldsymbol{L}, \boldsymbol{K})$ as

$$\begin{aligned} \phi(\boldsymbol{\epsilon}, \boldsymbol{q}) &= \frac{1}{2}\boldsymbol{\epsilon} : \boldsymbol{C} : \boldsymbol{\epsilon} + \boldsymbol{\epsilon} : \boldsymbol{H} \cdot \boldsymbol{q} + \frac{1}{2}\boldsymbol{q} \cdot \boldsymbol{R} \cdot \boldsymbol{q}, \\ \psi(\boldsymbol{\sigma}, \boldsymbol{p}) &= \frac{1}{2}\boldsymbol{\sigma} : \boldsymbol{D} : \boldsymbol{\sigma} + \boldsymbol{\sigma} : \boldsymbol{L} \cdot \boldsymbol{p} + \frac{1}{2}\boldsymbol{p} \cdot \boldsymbol{K} \cdot \boldsymbol{p}. \end{aligned} \tag{19}$$

In this form, ϕ or ψ is positive-definite and convex, as shown by Lothe and Barnett (1977).

For given $(\boldsymbol{E}, \boldsymbol{Q})$ or $(\boldsymbol{\Sigma}, \boldsymbol{P})$, the macropotentials are then expressed in terms of the effective moduli $(\overline{\boldsymbol{C}}^G, \overline{\boldsymbol{H}}^G, \overline{\boldsymbol{R}}^G)$ which satisfy

$$\langle\boldsymbol{\sigma}^G\rangle = \overline{\boldsymbol{C}}^G : \boldsymbol{E} + \overline{\boldsymbol{H}}^G \cdot \boldsymbol{Q}, \qquad \langle\boldsymbol{p}^G\rangle = \left(\overline{\boldsymbol{H}}^G\right)^{\mathrm{T}} : \boldsymbol{E} + \overline{\boldsymbol{R}}^G \cdot \boldsymbol{Q},$$

or in terms of $(\overline{\boldsymbol{D}}^G, \overline{\boldsymbol{L}}^G, \overline{\boldsymbol{R}}^G)$ which satisfy

$$\langle\boldsymbol{\epsilon}^G\rangle = \overline{\boldsymbol{D}}^G : \boldsymbol{\Sigma} + \overline{\boldsymbol{L}}^G \cdot \boldsymbol{P}, \qquad \langle\boldsymbol{q}^G\rangle = \left(\overline{\boldsymbol{L}}^G\right)^{\mathrm{T}} : \boldsymbol{\Sigma} + \overline{\boldsymbol{K}}^G \cdot \boldsymbol{P},$$

as follows:

$$\begin{aligned} \Phi^G(\boldsymbol{E}, \boldsymbol{Q}) &= \frac{1}{2}\boldsymbol{E} : \overline{\boldsymbol{C}}^G : \boldsymbol{E} + \boldsymbol{E} : \overline{\boldsymbol{H}}^G \cdot \boldsymbol{Q} + \frac{1}{2}\boldsymbol{Q} \cdot \overline{\boldsymbol{R}}^G \cdot \boldsymbol{Q}, \\ \Psi^G(\boldsymbol{\Sigma}, \boldsymbol{P}) &= \frac{1}{2}\boldsymbol{\Sigma} : \overline{\boldsymbol{D}}^G : \boldsymbol{\Sigma} + \boldsymbol{\Sigma} : \overline{\boldsymbol{L}}^G \cdot \boldsymbol{P} + \frac{1}{2}\boldsymbol{P} \cdot \overline{\boldsymbol{K}}^G \cdot \boldsymbol{P}; \end{aligned} \tag{20}$$

see Fig. 2 for the choice of field variables used in determining $(\overline{\boldsymbol{C}}^G, \overline{\boldsymbol{H}}^G, \overline{\boldsymbol{R}}^G)$ or $(\overline{\boldsymbol{D}}^G, \overline{\boldsymbol{L}}^G, \overline{\boldsymbol{K}}^G)$. Here, superscript G emphasizes that quantities are for general boundary data. It should be recalled that the effective moduli defined through the relations between $(\langle\boldsymbol{\epsilon}\rangle, \langle\boldsymbol{q}\rangle)$ and $(\langle\boldsymbol{\sigma}\rangle, \langle\boldsymbol{p}\rangle)$ satisfy Eq. (20) if the boundary data are of the Hill-type. In general, however, the moduli defined through the energy relations do not coincide with the moduli defined directly by relating the average field variables; see Nemat-Nasser and Hori (1993). In what follows, we assume that the boundary data are of the Hill-type.

There are various Hill-type boundary data satisfying $(\langle\boldsymbol{\epsilon}\rangle, \langle\boldsymbol{q}\rangle) = (\boldsymbol{E}, \boldsymbol{Q})$ or $(\langle\boldsymbol{\sigma}\rangle, \langle\boldsymbol{p}\rangle) = (\boldsymbol{\Sigma}, \boldsymbol{P})$ for given $(\boldsymbol{E}, \boldsymbol{Q})$ or $(\boldsymbol{\Sigma}, \boldsymbol{P})$. The resulting macropotentials necessarily depend on the boundary data, as do the resulting effective moduli. Theorems I and II provide strict bounds for this class of effective moduli, through the following inequalities:

$$\begin{aligned} &\frac{1}{2}\boldsymbol{E} : \overline{\boldsymbol{C}}^{\Sigma P} : \boldsymbol{E} + \boldsymbol{E} : \overline{\boldsymbol{H}}^{\Sigma P} \cdot \boldsymbol{Q} + \frac{1}{2}\boldsymbol{Q} \cdot \overline{\boldsymbol{R}}^{\Sigma P} \cdot \boldsymbol{Q} < \frac{1}{2}\boldsymbol{E} : \overline{\boldsymbol{C}}^G : \boldsymbol{E} + \boldsymbol{E} : \overline{\boldsymbol{H}}^G \cdot \boldsymbol{Q} + \frac{1}{2}\boldsymbol{Q} \cdot \overline{\boldsymbol{R}}^G \cdot \boldsymbol{Q}, \\ &\frac{1}{2}\boldsymbol{\Sigma} : \overline{\boldsymbol{D}}^{EQ} : \boldsymbol{\Sigma} + \boldsymbol{\Sigma} : \overline{\boldsymbol{L}}^{EQ} \cdot \boldsymbol{P} + \frac{1}{2}\boldsymbol{P} \cdot \overline{\boldsymbol{K}}^{EQ} \cdot \boldsymbol{P} < \frac{1}{2}\boldsymbol{\Sigma} : \overline{\boldsymbol{D}}^G : \boldsymbol{\Sigma} + \boldsymbol{\Sigma} : \overline{\boldsymbol{L}}^G \cdot \boldsymbol{P} + \frac{1}{2}\boldsymbol{P} \cdot \overline{\boldsymbol{K}}^G \cdot \boldsymbol{P}, \end{aligned} \tag{21}$$

for any pair of $(\boldsymbol{E}, \boldsymbol{Q})$ or $(\boldsymbol{\Sigma}, \boldsymbol{P})$, where, again, superscript EQ or ΣP emphasizes that the corresponding quantities are for the uniform boundary data (9) or (10), respectively.

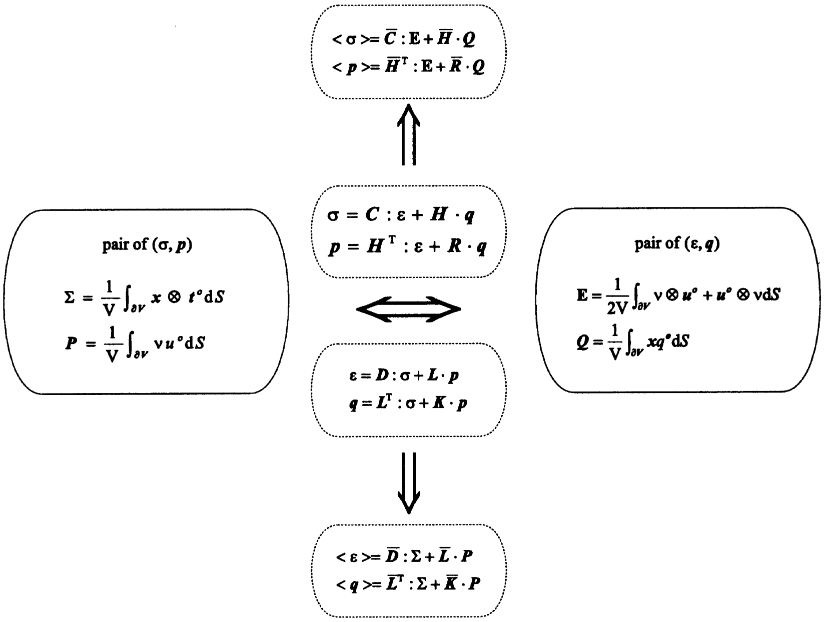

Fig. 2. Pair of field variables used in deriving universal inequalities.

Combining the above two inequalities, we obtain

$$\frac{1}{2}\boldsymbol{E}:\overline{\boldsymbol{C}}^{\Sigma P}:\boldsymbol{E}+\boldsymbol{E}:\overline{\boldsymbol{H}}^{\Sigma P}\cdot\boldsymbol{Q}+\frac{1}{2}\boldsymbol{Q}\cdot\overline{\boldsymbol{R}}^{\Sigma P}\cdot\boldsymbol{Q}<\frac{1}{2}\boldsymbol{E}:\overline{\boldsymbol{C}}^{G}:\boldsymbol{E}+\boldsymbol{E}:\overline{\boldsymbol{H}}^{G}\cdot\boldsymbol{Q}+\frac{1}{2}\boldsymbol{Q}\cdot\overline{\boldsymbol{R}}^{G}\cdot\boldsymbol{Q}<\frac{1}{2}\boldsymbol{E}:\overline{\boldsymbol{C}}^{EQ}:\boldsymbol{E}$$
$$+\boldsymbol{E}:\overline{\boldsymbol{H}}^{EQ}\cdot\boldsymbol{Q}+\frac{1}{2}\boldsymbol{Q}\cdot\overline{\boldsymbol{R}}^{EQ}\cdot\boldsymbol{Q}. \tag{22}$$

Similar inequalities are obtained in terms of the compliance tensors. These are the *universal inequalities* for general coupled mechanical/non-mechanical problems. When the moduli are defined through the energy relations, then they are valid for *any general* boundary data, not necessarily of the Hill-type. They thus hold for a finite volume as well as for an RVE.

An RVE used to compute the effective moduli can be regarded to be representing a statistically homogeneous solid, if the difference of the left side and the right side of inequality (22) is negligibly small, i.e., if

$$\frac{\Phi^{EQ}(\boldsymbol{E},\boldsymbol{Q})-\Phi^{\Sigma P}(\boldsymbol{E},\boldsymbol{Q})}{\Phi^{EQ}(\boldsymbol{E},\boldsymbol{Q})}\ll 1, \tag{23}$$

where

$$\Phi^{(\cdot)}(\boldsymbol{E},\boldsymbol{Q})=\frac{1}{2}\boldsymbol{E}:\overline{\boldsymbol{C}}^{(\cdot)}:\boldsymbol{E}+\boldsymbol{E}:\overline{\boldsymbol{H}}^{(\cdot)}\cdot\boldsymbol{Q}+\frac{1}{2}\boldsymbol{Q}\cdot\overline{\boldsymbol{R}}^{(\cdot)}\cdot\boldsymbol{Q}.$$

4. Hashin–Shtrikman variational principles for piezoelectricity

In this subsection, the Hashin–Shtrikman variational principles are generalized and applied to the coupled piezoelectricity problems, taking the following three steps.

1. Assume the Hill-type boundary data for the RVE.
2. Homogenize the RVE using the equivalent inclusion method.
3. Establish functionals whose Euler equations coincide with the consistency conditions of the equivalent inclusion method.

From the variational principles computable upper or lower bounds for the effective moduli are then obtained.

4.1. Generalized Hashin–Shtrikman variational principles

Suppose that an RVE of volume V and boundary ∂V is subjected to Hill-type boundary conditions; see Eq. (8). For the Hill-type boundary data, we have

$$\int_{\partial V} (\boldsymbol{t}^d \cdot \boldsymbol{u}^d + q^d p^d)\, \mathrm{d}S = 0, \tag{24}$$

where $(\boldsymbol{u}^d, \boldsymbol{t}^d) = (\boldsymbol{u} - \boldsymbol{x} \cdot \langle \boldsymbol{\epsilon} \rangle, \boldsymbol{v} \cdot (\boldsymbol{\sigma} - \langle \boldsymbol{\sigma} \rangle))$ and $(p^d, q^d) = (p - \boldsymbol{x} \cdot \langle \boldsymbol{p} \rangle, \boldsymbol{v} \cdot (\boldsymbol{q} - \langle \boldsymbol{q} \rangle))$. For simplicity, Eq. (24) is called the *admissibility condition*. When Eq. (24) is satisfied, then the effective moduli defined through the average energy relations coincide with those obtained by directly relating the averaging field variables. The quantities $\boldsymbol{\epsilon}^d$, $\boldsymbol{\sigma}^d$, $\boldsymbol{p}^d$, and $\boldsymbol{q}^d$ are called the *disturbance* strain, stress, electric field, and electric displacement, respectively.

The boundary-value problem of the heterogeneous RVE with the Hill-type boundary data satisfying Eq. (24), is solved using the equivalent inclusion method. To this end, a homogeneous body, denoted by V^0, with constant reference moduli, $(\boldsymbol{C}^0, \boldsymbol{H}^0, \boldsymbol{R}^0)$, is considered. Within V^0, suitable eigenstress and eigen-electric field, $(\boldsymbol{\sigma}^*, \boldsymbol{p}^*)$, are introduced such that the resulting stress, strain, electric field, and electric displacement in this homogeneous body coincide with those of the original heterogeneous RVE. The stress and electric field in the homogeneous V^0 are given by

$$\begin{aligned} \boldsymbol{\sigma}(\boldsymbol{x}) &= \boldsymbol{C}^0 : \boldsymbol{\epsilon}(\boldsymbol{x}) + \boldsymbol{H}^0 \cdot \boldsymbol{q}(\boldsymbol{x}) + \boldsymbol{\sigma}^*(\boldsymbol{x}), \\ \boldsymbol{p}(\boldsymbol{x}) &= (\boldsymbol{H}^0)^{\mathrm{T}} : \boldsymbol{\epsilon}(\boldsymbol{x}) + \boldsymbol{R}^0 \cdot \boldsymbol{q}(\boldsymbol{x}) + \boldsymbol{p}^*(\boldsymbol{x}), \end{aligned} \tag{25}$$

where the dependence on the variable $\boldsymbol{x}$ is shown explicitly. For the field variables in the homogeneous V^0 to coincide with those of the original heterogeneous V, we must have the following *consistency conditions*:

$$\begin{aligned} \boldsymbol{C}(\boldsymbol{x}) : \boldsymbol{\epsilon}(\boldsymbol{x}) + \boldsymbol{H}(\boldsymbol{x}) \cdot \boldsymbol{q}(\boldsymbol{x}) &= \boldsymbol{C}^0 : \boldsymbol{\epsilon}(\boldsymbol{x}) + \boldsymbol{H}^0 \cdot \boldsymbol{q}(\boldsymbol{x}) + \boldsymbol{\sigma}^*(\boldsymbol{x}), \\ \boldsymbol{H}^{\mathrm{T}}(\boldsymbol{x}) : \boldsymbol{\epsilon}(\boldsymbol{x}) + \boldsymbol{R}(\boldsymbol{x}) \cdot \boldsymbol{q}(\boldsymbol{x}) &= (\boldsymbol{H}^0)^{\mathrm{T}} : \boldsymbol{\epsilon}(\boldsymbol{x}) + \boldsymbol{R}^0 \cdot \boldsymbol{q}(\boldsymbol{x}) + \boldsymbol{p}^*(\boldsymbol{x}). \end{aligned} \tag{26}$$

For given $(\boldsymbol{\sigma}^*, \boldsymbol{p}^*)$, the solution of the boundary value problem for V^0 can be (formally) expressed in terms of suitable Green's functions. In view of Eq. (25), the governing equations for the mechanical displacement and the electric potential fields, $(\boldsymbol{u}, u)$, are

$$\begin{aligned} &\nabla \cdot (\boldsymbol{C}^{0\prime} : (\nabla \otimes \boldsymbol{u}(\boldsymbol{x})) - \nabla \cdot (\boldsymbol{L}^{0\prime} \cdot (\nabla u(\boldsymbol{x})) + \boldsymbol{b}(\boldsymbol{x}) = 0, \\ &- \nabla \cdot ((\boldsymbol{L}^{0\prime})^{\mathrm{T}} : (\nabla \otimes \boldsymbol{u}(\boldsymbol{x}))) - \nabla \cdot (\boldsymbol{K}^{0\prime} \cdot (\nabla u(\boldsymbol{x})) + c(\boldsymbol{x}) = 0, \end{aligned} \tag{27}$$

where $\boldsymbol{C}^{0\prime} = \boldsymbol{C}^0 - \boldsymbol{H}^0 \cdot \boldsymbol{K}^{0\prime} \cdot (\boldsymbol{H}^0)^{\mathrm{T}}$, $\boldsymbol{K}^{0\prime} = (\boldsymbol{R}^0)^{-1}$, and $\boldsymbol{L}^{0\prime} = \boldsymbol{H}^0 \cdot \boldsymbol{K}^{0\prime}$, and $\boldsymbol{b}$ and c are body forces and electric charges which are produced by $(\boldsymbol{\sigma}^*, \boldsymbol{p}^*)$, as

$$\boldsymbol{b}(\boldsymbol{x}) = \nabla \cdot (\boldsymbol{\sigma}^*(\boldsymbol{x}) - \boldsymbol{L}^{0\prime} \cdot \boldsymbol{p}^*(\boldsymbol{x})), \qquad c(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{K}^{0\prime} \cdot \boldsymbol{p}^*(\boldsymbol{x})).$$

In terms of the Green's functions that correspond to the volume V, the solution $(\boldsymbol{u}, u)$ is formally expressed as

$$\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{x}\cdot\boldsymbol{E} + \boldsymbol{u}^d(\boldsymbol{x}), \qquad u(\boldsymbol{x}) = \boldsymbol{x}\cdot\boldsymbol{P} + u^d(\boldsymbol{x}),$$

where

$$\boldsymbol{u}^d(\boldsymbol{x}) = \int_V \boldsymbol{G}^2(\boldsymbol{x},\boldsymbol{y})\cdot\boldsymbol{b}(\boldsymbol{y}) + \boldsymbol{G}^1(\boldsymbol{x},\boldsymbol{y})c(\boldsymbol{y})\,\mathrm{d}V_y,$$
$$u^d(\boldsymbol{x}) = \int_V \boldsymbol{g}^2(\boldsymbol{x},\boldsymbol{y})\cdot\boldsymbol{b}(\boldsymbol{y}) + g^1(\boldsymbol{x},\boldsymbol{y})c(\boldsymbol{y})\,\mathrm{d}V_y,$$

and $(\boldsymbol{E},\boldsymbol{P})$ are the average strain and electric field. The Green's functions, $(\boldsymbol{G}^2,\boldsymbol{g}^2)$ and $(\boldsymbol{G}^1,g^1)$, yield the disturbance displacement and electric potential, respectively, due to unit body force and electric charge. These Green's functions depend on the shape of the boundary of V. The strain and the electric displacement in Eq. (26) are now expressed as $(\boldsymbol{\epsilon},\boldsymbol{q}) = (\boldsymbol{E}+\boldsymbol{\epsilon}^d, \boldsymbol{Q}+\boldsymbol{q}^d)$, where

$$\boldsymbol{\epsilon}^d(\boldsymbol{x}) = -\boldsymbol{\Gamma}(\boldsymbol{x};\boldsymbol{\sigma}^*,\boldsymbol{p}^*), \qquad \boldsymbol{q}^d(\boldsymbol{x}) = -\gamma(\boldsymbol{x};\boldsymbol{\sigma}^*,\boldsymbol{p}^*).$$

Here, $(\boldsymbol{\Gamma},\gamma)$ are integral operators which are defined by $(\boldsymbol{G}^2,\boldsymbol{g}^2)$ and $(\boldsymbol{G}^1,g^1)$, and give the disturbance strain and electric displacement. The consistency conditions (26) are rewritten as

$$\begin{aligned}&\Delta\boldsymbol{C}^{-1}(\boldsymbol{x}):\boldsymbol{\sigma}^*(\boldsymbol{x}) + \Delta\boldsymbol{H}^{-1}(\boldsymbol{x})\cdot\boldsymbol{p}^*(\boldsymbol{x}) + \boldsymbol{\Gamma}(\boldsymbol{x};\boldsymbol{\sigma}^*,\boldsymbol{p}^*) - \boldsymbol{E} = 0,\\ &\Delta\boldsymbol{H}^{-\mathrm{T}}(\boldsymbol{x}):\boldsymbol{\sigma}^*(\boldsymbol{x}) + \Delta\boldsymbol{R}^{-1}(\boldsymbol{x})\cdot\boldsymbol{p}^*(\boldsymbol{x}) + \gamma(\boldsymbol{x};\boldsymbol{\sigma}^*,\boldsymbol{p}^*) - \boldsymbol{Q} = 0,\end{aligned} \tag{28}$$

where

$$\begin{aligned}\Delta\boldsymbol{C}(\boldsymbol{x}) &= \left(\boldsymbol{C}(\boldsymbol{x}) - \boldsymbol{C}^0\right) - \left(\boldsymbol{H}(\boldsymbol{x}) - \boldsymbol{H}^0\right)\cdot\left(\boldsymbol{R}(\boldsymbol{x}) - \boldsymbol{R}^0\right)^{-1}\cdot\left(\boldsymbol{H}(\boldsymbol{x}) - \boldsymbol{H}^0\right)^{\mathrm{T}},\\ \Delta\boldsymbol{H}(\boldsymbol{x}) &= -\Delta\boldsymbol{C}^{-1}(\boldsymbol{x}):\left(\boldsymbol{H}(\boldsymbol{x}) - \boldsymbol{H}^0\right)\cdot\left(\boldsymbol{R}(\boldsymbol{x}) - \boldsymbol{R}^0\right)^{-1},\\ \Delta\boldsymbol{R}(\boldsymbol{x}) &= \left(\boldsymbol{R}(\boldsymbol{x}) - \boldsymbol{R}^0\right) - \left(\boldsymbol{H}(\boldsymbol{x}) - \boldsymbol{H}^0\right)^{\mathrm{T}}:\left(\boldsymbol{C}(\boldsymbol{x}) - \boldsymbol{C}^0\right)^{-1}:\left(\boldsymbol{H}(\boldsymbol{x}) - \boldsymbol{H}^0\right).\end{aligned}$$

Eqs. (28) are integral equations for $(\boldsymbol{\sigma}^*,\boldsymbol{p}^*)$. The solution of the boundary-value problem for the heterogeneous RVE is given by the solution of the integral equations Eq. (28).

Taking advantage of Eq. (24), we define a functional for arbitrary eigenstress and eigen-electric field, $(\boldsymbol{s}^*,\boldsymbol{\phi}^*)$, such that the corresponding Euler equations coincide with Eq. (28). This functional is given by

$$\begin{aligned}J(\boldsymbol{s}^*,\boldsymbol{\phi}^*;\boldsymbol{\Gamma},\gamma;\boldsymbol{E},\boldsymbol{Q}) = \frac{1}{2}\big\langle \boldsymbol{s}^*:\left(\Delta\boldsymbol{C}^{-1}:\boldsymbol{s}^* + \Delta\boldsymbol{H}^{-1}\cdot\boldsymbol{\phi}^* + \boldsymbol{\Gamma}(\boldsymbol{s}^*,\boldsymbol{\phi}^*)\right)\\ +\boldsymbol{\phi}^*\cdot\left(\Delta\boldsymbol{H}^{-\mathrm{T}}:\boldsymbol{s}^* + \Delta\boldsymbol{R}^{-1}\cdot\boldsymbol{\phi}^* + \gamma(\boldsymbol{s}^*,\boldsymbol{\phi}^*)\right)\big\rangle - \left(\langle\boldsymbol{s}^*\rangle:\boldsymbol{E} + \langle\boldsymbol{\phi}^*\rangle\cdot\boldsymbol{Q}\right).\end{aligned} \tag{29}$$

Indeed, since Eq. (24) leads to $\delta(\langle\boldsymbol{s}^*:\boldsymbol{\Gamma} + \boldsymbol{\phi}^*\cdot\gamma\rangle) = 2\langle\delta\boldsymbol{s}^*:\boldsymbol{\Gamma} + \delta\boldsymbol{\phi}^*\cdot\gamma\rangle$, vanishing of the first variation of J for arbitrary variations $(\delta\boldsymbol{s}^*,\delta\boldsymbol{\phi}^*)$ yields Eq. (28), i.e.,

$$\big\langle\delta\boldsymbol{s}^*:\left(\Delta\boldsymbol{C}^{-1}:\boldsymbol{s}^* + \Delta\boldsymbol{H}^{-1}\cdot\boldsymbol{\phi}^* + \boldsymbol{\Gamma} - \boldsymbol{E}\right) + \delta\boldsymbol{\phi}^*\cdot\left(\Delta\boldsymbol{H}^{-\mathrm{T}}:\boldsymbol{s}^* + \Delta\boldsymbol{R}^{-1}\cdot\boldsymbol{\phi}^* + \gamma - \boldsymbol{Q}\right)\big\rangle = 0.$$

Like a functional used in the Hashin–Shtrikman variational principles, the above defined J has the following two properties:

1. The stationary value of J gives the effective moduli of V.
2. The stationary value becomes the minimum when $\left(\boldsymbol{C}^0,\boldsymbol{H}^0,\boldsymbol{R}^0\right)$ are chosen such that the set $(\boldsymbol{C}^0-\boldsymbol{C},\boldsymbol{H}^0-\boldsymbol{H},\boldsymbol{R}^0-\boldsymbol{R})$ is [9] positive-definite.

[9] If the scalar quantity $\boldsymbol{\epsilon}:\boldsymbol{C}:\boldsymbol{\epsilon} + 2\boldsymbol{\epsilon}:\boldsymbol{H}\cdot\boldsymbol{q} + \boldsymbol{q}\cdot\boldsymbol{R}\cdot\boldsymbol{q}$ is positive for any $(\boldsymbol{\epsilon},\boldsymbol{q}) \neq (\boldsymbol{0},\boldsymbol{0})$, then the set $(\boldsymbol{C},\boldsymbol{H},\boldsymbol{R})$ is called positive-definite.

The proof of the first property is straightforward: since the exact eigenstress and eigen-electric fields, $(\boldsymbol{\sigma}^*, \boldsymbol{p}^*)$, that satisfy Eq. (28), render J stationary, the stationary value is

$$J(\boldsymbol{\sigma}^*, \boldsymbol{p}^*) = -\frac{1}{2}\langle \boldsymbol{\sigma}^* : \boldsymbol{E} + \boldsymbol{p}^* \cdot \boldsymbol{Q} \rangle = \frac{1}{2}\boldsymbol{E} : (\boldsymbol{C}^0 - \overline{\boldsymbol{C}}^G) : \boldsymbol{E} + \boldsymbol{E} : (\boldsymbol{H}^0 - \overline{\boldsymbol{H}}^G) \cdot \boldsymbol{Q} + \frac{1}{2}\boldsymbol{Q} \cdot (\boldsymbol{R} - \overline{\boldsymbol{R}}^G) \cdot \boldsymbol{Q}, \tag{30}$$

where $(\overline{\boldsymbol{C}}^G, \overline{\boldsymbol{H}}^G, \overline{\boldsymbol{R}}^G)$ are the effective moduli which are defined through

$$\langle \boldsymbol{\sigma} \rangle = \overline{\boldsymbol{C}} : \boldsymbol{E} + \overline{\boldsymbol{H}} \cdot \boldsymbol{Q}, \qquad \langle \boldsymbol{p} \rangle = \overline{\boldsymbol{H}}^{\mathrm{T}} : \boldsymbol{\epsilon} + \overline{\boldsymbol{R}} \cdot \boldsymbol{Q}.$$

The second property is proved by using a fact that if $(\boldsymbol{C}^0 - \boldsymbol{C}, \boldsymbol{H}^0 - \boldsymbol{H}, \boldsymbol{R}^0 - \boldsymbol{R})$ is positive-definite, then the integral operators $(\boldsymbol{\Gamma}, \gamma)$ associated with the averaging operator $\langle\langle(.)\rangle\rangle$ produce a positive number for any $(\boldsymbol{s}^*, \boldsymbol{\phi}^*)$, i.e.,

$$\left\langle \boldsymbol{s}^* : \left(\Delta \boldsymbol{C}^{-1} : \boldsymbol{s}^* + \Delta \boldsymbol{H}^{-1} \cdot \boldsymbol{\phi}^* + \boldsymbol{\Gamma}\right) + \boldsymbol{\phi}^* : \left(\Delta \boldsymbol{H}^{-\mathrm{T}} : \boldsymbol{s}^* + \Delta \boldsymbol{R}^{-1} \cdot \boldsymbol{\phi}^* + \gamma\right) \right\rangle > 0.$$

This is because Eq. (24) leads to

$$\langle \boldsymbol{s}^* : \boldsymbol{\Gamma} + \boldsymbol{\phi}^* \cdot \gamma \rangle = \left\langle \boldsymbol{\Gamma} : \boldsymbol{C}^0 : \boldsymbol{\Gamma} + 2\boldsymbol{\Gamma} \cdot \boldsymbol{H}^0 : \gamma + \gamma \cdot \boldsymbol{R}^0 \cdot \gamma \right\rangle > 0,$$

when $(\boldsymbol{C}^0, \boldsymbol{H}^0, \boldsymbol{R}^0)$ are positive-definite.

The two properties of J lead to the following bound for the effective moduli:

$$\frac{1}{2}\boldsymbol{E} : (\boldsymbol{C}^0 - \overline{\boldsymbol{C}}^G) : \boldsymbol{E} + \boldsymbol{E} : (\boldsymbol{H}^0 - \overline{\boldsymbol{H}}^G) \cdot \boldsymbol{Q} + \frac{1}{2}\boldsymbol{Q} \cdot \left(\boldsymbol{R}^0 - \overline{\boldsymbol{R}}^G\right) \cdot \boldsymbol{Q} < J(\boldsymbol{s}^*, \boldsymbol{\phi}^*; \boldsymbol{\Gamma}, \gamma; \boldsymbol{E}, \boldsymbol{Q}). \tag{31}$$

Here, $(\boldsymbol{C}^0, \boldsymbol{H}^0, \boldsymbol{R}^0)$ is chosen such that $(\boldsymbol{C}^0 - \boldsymbol{C}, \boldsymbol{H}^0 - \boldsymbol{H}, \boldsymbol{R}^0 - \boldsymbol{R})$ is positive-definite.

An alternative functional and the related inequalities can be obtained by using the *dual* formulation, i.e., by switching $(\boldsymbol{\epsilon}, \boldsymbol{q})$ and $(\boldsymbol{\sigma}, \boldsymbol{p})$. When eigenstrain and eigen-electric displacement fields, $(\boldsymbol{\epsilon}^*, \boldsymbol{q}^*)$, are prescribed in the homogeneous V^0 instead of $(\boldsymbol{\sigma}^*, \boldsymbol{p}^*)$, the resulting disturbance stress and electric fields are formally expressed in terms of suitable integral operators as $\boldsymbol{\sigma}^d = -\boldsymbol{\Lambda}(\boldsymbol{\epsilon}^*, \boldsymbol{q}^*)$ and $\boldsymbol{p}^d = -\boldsymbol{\lambda}(\boldsymbol{\epsilon}^*, \boldsymbol{q}^*)$, where $(\boldsymbol{\Lambda}, \boldsymbol{\lambda})$ are determined by using the formal Green's functions $(\boldsymbol{G}^2, \boldsymbol{g}^2)$ and $(\boldsymbol{G}^1, g^1)$. The boundary-value problem for the heterogeneous V is now replaced by the integral equations of the consistency conditions for $(\boldsymbol{\epsilon}^*, \boldsymbol{q}^*)$,

$$\begin{aligned} &\Delta \boldsymbol{D}^{-1}(\boldsymbol{x}) : \boldsymbol{\epsilon}^*(\boldsymbol{x}) + \Delta \boldsymbol{L}^{-1}(\boldsymbol{x}) \cdot \boldsymbol{q}^*(\boldsymbol{x}) + \boldsymbol{\Lambda}(\boldsymbol{x}; \boldsymbol{\epsilon}^*, \boldsymbol{q}^*) - \boldsymbol{\Sigma} = 0, \\ &\Delta \boldsymbol{L}^{-1}(\boldsymbol{x}) : \boldsymbol{\epsilon}^*(\boldsymbol{x}) + \Delta \boldsymbol{K}^{-1}(\boldsymbol{x}) \cdot \boldsymbol{q}^*(\boldsymbol{x}) + \boldsymbol{\lambda}(\boldsymbol{x}; \boldsymbol{\epsilon}^*, \boldsymbol{q}^*) - \boldsymbol{P} = 0, \end{aligned} \tag{32}$$

where $(\boldsymbol{\Sigma}, \boldsymbol{P}) = (\langle \boldsymbol{\sigma} \rangle, \langle \boldsymbol{p} \rangle)$, and

$$\begin{aligned} \Delta \boldsymbol{D}(\boldsymbol{x}) &= \left(\boldsymbol{D}(\boldsymbol{x}) - \boldsymbol{D}^0\right) - \left(\boldsymbol{L}(\boldsymbol{x}) - \boldsymbol{L}^0\right) \cdot \left(\boldsymbol{K}(\boldsymbol{x}) - \boldsymbol{K}^0\right)^{-1} \cdot \left(\boldsymbol{L}(\boldsymbol{x}) - \boldsymbol{L}^0\right), \\ \Delta \boldsymbol{L}(\boldsymbol{x}) &= -\Delta \boldsymbol{D}^{-1}(\boldsymbol{x}) : \left(\boldsymbol{L}(\boldsymbol{x}) - \boldsymbol{L}^0\right) \cdot \left(\boldsymbol{K}(\boldsymbol{x}) - \boldsymbol{K}^0\right)^{-1}, \\ \Delta \boldsymbol{K}(\boldsymbol{x}) &= \left(\boldsymbol{K}(\boldsymbol{x}) - \boldsymbol{K}^0\right) - \left(\boldsymbol{L}(\boldsymbol{x}) - \boldsymbol{L}^0\right)^{\mathrm{T}} : \left(\boldsymbol{D}(\boldsymbol{x}) - \boldsymbol{D}^0\right)^{-1} : \left(\boldsymbol{L}(\boldsymbol{x}) - \boldsymbol{L}^0\right). \end{aligned}$$

Using the admissibility of the boundary data, Eq. (24), we can define a functional for arbitrary eigenstrain and eigen-electric displacement, $(\boldsymbol{e}^*, \boldsymbol{\psi}^*)$, such that the corresponding Euler equations coincide with the consistency conditions (32), as follows:

$$\begin{aligned} I(\boldsymbol{e}^*, \boldsymbol{\psi}^*; \boldsymbol{\Lambda}, \boldsymbol{\lambda}; \boldsymbol{\Sigma}, \boldsymbol{P}) = &\frac{1}{2}\left\langle \boldsymbol{e}^* : \left(\Delta \boldsymbol{D}^{-1} : \boldsymbol{e}^* + \Delta \boldsymbol{L}^{-1} \cdot \boldsymbol{\psi}^* + \boldsymbol{\Lambda}(\boldsymbol{e}^*, \boldsymbol{\psi}^*)\right) \right. \\ &\left. + \boldsymbol{\psi}^* \cdot \left(\Delta \boldsymbol{L}^{-\mathrm{T}} : \boldsymbol{e}^* + \Delta \boldsymbol{K}^{-1} \cdot \boldsymbol{\psi}^* + \gamma(\boldsymbol{e}^*, \boldsymbol{\psi}^*)\right) \right\rangle - (\boldsymbol{\Sigma} : \langle \boldsymbol{e}^* \rangle + \boldsymbol{P} \cdot \langle \boldsymbol{\psi}^* \rangle). \end{aligned} \tag{33}$$

This I is stationary for $(\boldsymbol{e}^*, \boldsymbol{\psi}^*) = (\boldsymbol{\epsilon}^*, \boldsymbol{q}^*)$, and the stationary value is

$$I(\boldsymbol{\epsilon}^*, \boldsymbol{q}^*) = -\frac{1}{2}\langle \boldsymbol{\epsilon}^* : \boldsymbol{\Sigma} + \boldsymbol{q}^* \cdot \boldsymbol{P} \rangle = \frac{1}{2}\boldsymbol{\Sigma} : (\boldsymbol{D}^0 - \overline{\boldsymbol{D}}^G) : \boldsymbol{\Sigma} + \boldsymbol{\Sigma} : (\boldsymbol{L}^0 - \overline{\boldsymbol{L}}^G) \cdot \boldsymbol{P} + \frac{1}{2}\boldsymbol{P} \cdot (\boldsymbol{K} - \overline{\boldsymbol{K}}^G) \cdot \boldsymbol{P}, \tag{34}$$

where $(\overline{\boldsymbol{D}}^G, \overline{\boldsymbol{L}}^G, \overline{\boldsymbol{K}}^G)$ are the effective moduli defined through

$$\langle \boldsymbol{\epsilon} \rangle = \overline{\boldsymbol{D}}^G : \boldsymbol{\Sigma} + \overline{\boldsymbol{L}}^G \cdot \boldsymbol{P}, \qquad \langle \boldsymbol{q} \rangle = \left(\overline{\boldsymbol{L}}^G\right)^{\mathrm{T}} : \boldsymbol{\Sigma} + \overline{\boldsymbol{K}}^G \cdot \boldsymbol{P}.$$

When $\left(\boldsymbol{D}^0 - \boldsymbol{D}, \boldsymbol{L}^0 - \boldsymbol{L}, \boldsymbol{K}^0 - \boldsymbol{K}\right)$ is positive-definite, the stationary value of I is the minimum, and hence the following bound for $\left(\overline{\boldsymbol{D}}^G, \overline{\boldsymbol{L}}^G, \overline{\boldsymbol{K}}^G\right)$ is obtained:

$$\frac{1}{2}\boldsymbol{\Sigma} : (\boldsymbol{D}^0 - \overline{\boldsymbol{D}}^G) : \boldsymbol{\Sigma} + \boldsymbol{\Sigma} : (\boldsymbol{L}^0 - \overline{\boldsymbol{L}}^G) \cdot \boldsymbol{P} + \frac{1}{2}\boldsymbol{P} \cdot \left(\boldsymbol{K}^0 - \overline{\boldsymbol{K}}^G\right) \cdot \boldsymbol{P} < I(\boldsymbol{e}^*, \boldsymbol{\psi}^*; \boldsymbol{\Lambda}, \boldsymbol{\lambda}; \boldsymbol{\Sigma}, \boldsymbol{P}). \tag{35}$$

The functional I is used to solve the same boundary-value problem for V as the functional J, and hence these two are related; for instance, the following equality holds when $(\boldsymbol{e}^*, \boldsymbol{\psi}^*)$ and $(\boldsymbol{\Sigma}, \boldsymbol{P})$ are given by $(-\left(\boldsymbol{D}^0 : \boldsymbol{s}^* + \boldsymbol{L}^0 \cdot \boldsymbol{\phi}^*\right), -(\left(\boldsymbol{L}^0\right)^{\mathrm{T}} : \boldsymbol{s}^* + \boldsymbol{K}^0 \cdot \boldsymbol{\phi}^*))$ and $(\boldsymbol{C}^0 : \boldsymbol{E} + \boldsymbol{H}^0 \cdot \boldsymbol{Q} + \langle \boldsymbol{s}^* \rangle, \left(\boldsymbol{H}^0\right)^{\mathrm{T}} : \boldsymbol{E} + \boldsymbol{R}^0 \cdot \boldsymbol{Q} + \langle \boldsymbol{\phi}^* \rangle)$:

$$\begin{aligned} I(\boldsymbol{e}^*, \boldsymbol{\psi}^*; \boldsymbol{\Lambda}, \boldsymbol{\lambda}; \boldsymbol{\Sigma}, \boldsymbol{P}) &- \left(\frac{1}{2}\boldsymbol{\Sigma} : \boldsymbol{D}^0 : \boldsymbol{\Sigma} + \boldsymbol{\Sigma} : \boldsymbol{L}^0 \cdot \boldsymbol{P} + \frac{1}{2}\boldsymbol{P} \cdot \boldsymbol{K}^0 \cdot \boldsymbol{P}\right) \\ &= J(\boldsymbol{s}^*, \boldsymbol{\phi}^*; \boldsymbol{\Gamma}, \boldsymbol{\gamma}; \boldsymbol{E}, \boldsymbol{Q}) - \left(\frac{1}{2}\boldsymbol{E} : \boldsymbol{C}^0 : \boldsymbol{E} + \boldsymbol{E} : \boldsymbol{H}^0 \cdot \boldsymbol{Q} + \frac{1}{2}\boldsymbol{Q} \cdot \boldsymbol{R}^0 \cdot \boldsymbol{Q}\right). \end{aligned} \tag{36}$$

Since $(\overline{\boldsymbol{D}}^G, \overline{\boldsymbol{L}}^G, \overline{\boldsymbol{K}}^G)$ are the inverse [10] of $(\overline{\boldsymbol{C}}^G, \overline{\boldsymbol{H}}^G, \overline{\boldsymbol{R}}^G)$ and the positive-definiteness of $(\boldsymbol{D}^0 - \boldsymbol{D}, \boldsymbol{L}^0 - \boldsymbol{L}, \boldsymbol{K}^0 - \boldsymbol{K})$ leads to the negative-definiteness of $\left(\boldsymbol{C}^0 - \boldsymbol{C}, \boldsymbol{H}^0 - \boldsymbol{H}, \boldsymbol{R}^0 - \boldsymbol{R}\right)$, two inequalities (31) and (35) now lead to upper or lower bounds for, say, $\left(\overline{\boldsymbol{C}}^G, \overline{\boldsymbol{H}}^G, \overline{\boldsymbol{R}}^G\right)$, as follows: if $(\boldsymbol{C}^0 - \boldsymbol{C}, \boldsymbol{H}^0 - \boldsymbol{H}, \boldsymbol{R}^0 - \boldsymbol{R})$ is positive- (negative-) definite, then

$$\begin{aligned} \frac{1}{2}\boldsymbol{E} : \overline{\boldsymbol{C}}^G : \boldsymbol{E} + \boldsymbol{E} : \overline{\boldsymbol{H}}^G \cdot \boldsymbol{Q} + \frac{1}{2}\boldsymbol{Q} \cdot \overline{\boldsymbol{R}}^G \cdot \boldsymbol{Q} &> (\text{or} <) - J(\boldsymbol{s}^*, \boldsymbol{\phi}^*; \boldsymbol{\Gamma}, \boldsymbol{\gamma}; \boldsymbol{E}, \boldsymbol{Q}) + \frac{1}{2}\boldsymbol{E} : \boldsymbol{C}^0 : \boldsymbol{E} \\ &+ \boldsymbol{E} : \boldsymbol{H}^0 \cdot \boldsymbol{Q} + \frac{1}{2}\boldsymbol{Q} \cdot \boldsymbol{R}^0 \cdot \boldsymbol{Q}. \end{aligned} \tag{37}$$

4.2. Consequence of universal theorems

In general, it may not be easy to explicitly determine Green's functions, $(\boldsymbol{G}^2, \boldsymbol{g}^2)$ and $(\boldsymbol{G}^1, g^1)$, and the associated integral operators, $(\boldsymbol{\Gamma}, \boldsymbol{\gamma})$ or $(\boldsymbol{\Lambda}, \boldsymbol{\lambda})$, for a finite region V. However, using Theorems I and II of Section 3, computable bounds are obtained in terms of the integral operators, $(\boldsymbol{\Gamma}^\infty, \boldsymbol{\gamma}^\infty)$ or $(\boldsymbol{\Lambda}^\infty, \boldsymbol{\lambda}^\infty)$, defined from the Green's functions, $(\boldsymbol{G}^{\infty 2}, \boldsymbol{g}^{\infty 2})$ and $(\boldsymbol{G}^{\infty 1}, g^{\infty 1})$, of an infinitely extended homogeneous domain. These bounds are established in two steps: first we consider the uniform boundary data and apply Theorems I and II, and then we relate the resulting bounds to those obtained by applying the integral operators of the infinite homogeneous domain.

First, consider a case when the RVE is subjected to the uniform boundary conditions given by Eq. (9). The resulting strain and electric displacement are $(\boldsymbol{\epsilon}^{EQ}, \boldsymbol{q}^{EQ})$, with the average values $(\boldsymbol{E}, \boldsymbol{Q})$. Theorem II now yields the following inequality:

[10] The inverse means that if $\left(\overline{\boldsymbol{D}}^G, \overline{\boldsymbol{L}}^G, \overline{\boldsymbol{K}}^G\right)$ satisfy $\boldsymbol{E} = \overline{\boldsymbol{D}}^G : \boldsymbol{\Sigma} + \overline{\boldsymbol{L}}^G \cdot \boldsymbol{P}$ and $\boldsymbol{Q} = \left(\overline{\boldsymbol{L}}^G\right)^{\mathrm{T}} : \boldsymbol{\Sigma} + \overline{\boldsymbol{K}}^G \cdot \boldsymbol{P}$, then $(\overline{\boldsymbol{C}}^G, \overline{\boldsymbol{H}}^G, \overline{\boldsymbol{R}}^G)$ yield $\boldsymbol{\Sigma} = \overline{\boldsymbol{C}}^G : \boldsymbol{E} + \overline{\boldsymbol{H}}^G \cdot \boldsymbol{Q}$ and $\boldsymbol{P} = (\overline{\boldsymbol{H}}^G)^{\mathrm{T}} : \boldsymbol{E} + \overline{\boldsymbol{R}}^G \cdot \boldsymbol{Q}$.

$$\left\langle \frac{1}{2}\boldsymbol{\epsilon}^{EQ}:\boldsymbol{C}:\boldsymbol{\epsilon}^{EQ}+\boldsymbol{\epsilon}^{EQ}:\boldsymbol{H}\cdot\boldsymbol{q}^{EQ}+\frac{1}{2}\boldsymbol{q}^{EQ}\cdot\boldsymbol{R}\cdot\boldsymbol{q}^{EQ}\right\rangle < \left\langle \frac{1}{2}\left(\boldsymbol{E}+\boldsymbol{\epsilon}^{d}\right):\boldsymbol{C}:\left(\boldsymbol{E}+\boldsymbol{\epsilon}^{d}\right)\right.$$
$$\left. +\left(\boldsymbol{E}+\boldsymbol{\epsilon}^{d}\right):\boldsymbol{H}\cdot\left(\boldsymbol{Q}+\boldsymbol{q}^{d}\right)+\frac{1}{2}\left(\boldsymbol{Q}+\boldsymbol{q}^{d}\right)\cdot\boldsymbol{R}\cdot\left(\boldsymbol{Q}+\boldsymbol{q}^{d}\right)\right\rangle. \tag{38}$$

A computable bound is obtained by combining this inequality with the inequalities (37).

Next, let $\left(\boldsymbol{C}^0,\boldsymbol{H}^0,\boldsymbol{R}^0\right)$ be constant reference moduli such that $\left(\boldsymbol{C}-\boldsymbol{C}^0,\boldsymbol{H}-\boldsymbol{H}^0,\boldsymbol{R}-\boldsymbol{R}^0\right)$ is negative-definite, i.e., for any pair of $(\boldsymbol{\epsilon},\boldsymbol{q})$ and $(\boldsymbol{\epsilon}',\boldsymbol{q}')$,

$$0>\frac{1}{2}(\boldsymbol{\epsilon}-\boldsymbol{\epsilon}'):\left(\boldsymbol{C}-\boldsymbol{C}^0\right):(\boldsymbol{\epsilon}-\boldsymbol{\epsilon}')+(\boldsymbol{\epsilon}-\boldsymbol{\epsilon}'):\left(\boldsymbol{H}-\boldsymbol{H}^0\right)\cdot(\boldsymbol{q}-\boldsymbol{q}')+\frac{1}{2}(\boldsymbol{q}-\boldsymbol{q}')\cdot\left(\boldsymbol{R}-\boldsymbol{R}^0\right)\cdot(\boldsymbol{q}-\boldsymbol{q}').$$

If $(\boldsymbol{\epsilon}',\boldsymbol{q}')$ are replaced by $\left(\Delta\boldsymbol{C}^{-1}:\boldsymbol{s}^*+\Delta\boldsymbol{H}^{-1}\cdot\boldsymbol{\phi}^*,\Delta\boldsymbol{H}^{-\mathrm{T}}:\boldsymbol{s}^*+\Delta\boldsymbol{R}^{-1}\cdot\boldsymbol{\phi}^*\right)$ with arbitrary $(\boldsymbol{s}^*,\boldsymbol{\phi}^*)$, the average of the above inequality taken over V^0 yields

$$0>\left\langle \frac{1}{2}\boldsymbol{\epsilon}:\left(\boldsymbol{C}-\boldsymbol{C}^0\right):\boldsymbol{\epsilon}+\boldsymbol{\epsilon}:\left(\boldsymbol{H}-\boldsymbol{H}^0\right)\cdot\boldsymbol{q}+\frac{1}{2}\boldsymbol{q}\cdot\left(\boldsymbol{R}-\boldsymbol{R}^0\right)\cdot\boldsymbol{q}-(\boldsymbol{s}^*:\boldsymbol{\epsilon}+\boldsymbol{\phi}^*\cdot\boldsymbol{q})\right.$$
$$\left.+\frac{1}{2}\boldsymbol{s}^*:\Delta\boldsymbol{C}^{-1}:\boldsymbol{s}^*+\boldsymbol{s}^*:\Delta\boldsymbol{H}^{-1}\cdot\boldsymbol{\phi}^*+\frac{1}{2}\boldsymbol{\phi}^*\cdot\Delta\boldsymbol{R}^{-1}\cdot\boldsymbol{\phi}^*\right\rangle.$$

Hence, comparing this inequality with the right side of Eq. (38), we obtain

$$\left\langle \frac{1}{2}\boldsymbol{\epsilon}^{EQ}:\boldsymbol{C}:\boldsymbol{\epsilon}^{EQ}+\boldsymbol{\epsilon}^{EQ}:\boldsymbol{H}\cdot\boldsymbol{q}^{EQ}+\frac{1}{2}\boldsymbol{q}^{EQ}\cdot\boldsymbol{R}\cdot\boldsymbol{q}^{EQ}\right\rangle<\frac{1}{2}\boldsymbol{E}:\boldsymbol{C}^0:\boldsymbol{E}+\boldsymbol{E}:\boldsymbol{H}^0\cdot\boldsymbol{Q}$$
$$+\frac{1}{2}\boldsymbol{Q}\cdot\boldsymbol{R}\cdot\boldsymbol{Q}-\frac{1}{2}\left\langle\left(\boldsymbol{s}^*:\left(\Delta\boldsymbol{C}^{-1}:\boldsymbol{s}^*+\Delta\boldsymbol{H}^{-1}\cdot\boldsymbol{\phi}^*\right)-\boldsymbol{s}^*:\left(\boldsymbol{\epsilon}^d+2\boldsymbol{E}\right)\right.\right.$$
$$\left.\left.+\boldsymbol{\phi}^*\cdot\left(\Delta\boldsymbol{H}^{-1}:\boldsymbol{s}^*+\Delta\boldsymbol{R}^{-1}\cdot\boldsymbol{\phi}^*\right)-\boldsymbol{\phi}^*\cdot\left(\boldsymbol{q}^d+2\boldsymbol{Q}\right)\right)\right\rangle+\left\langle\frac{1}{2}\boldsymbol{\sigma}^d:\boldsymbol{\epsilon}^d+\frac{1}{2}\boldsymbol{q}^d\cdot\boldsymbol{p}^d\right\rangle. \tag{39}$$

Now, we evaluate the disturbance strain and electric displacement using integral operators, $(\boldsymbol{\Gamma}^\infty,\gamma^\infty)$, associated with the Green's functions of the homogeneous infinite domain. As in the case of the uncoupled problems, the following relations hold for any arbitrary *ellipsoidal* RVE:

$$(\langle-\boldsymbol{\Gamma}^\infty\rangle,\langle-\gamma^\infty\rangle)=(0,0), \tag{40}$$
$$\left(\left\langle-\boldsymbol{C}^0:\boldsymbol{\Gamma}^\infty-\boldsymbol{H}^0\cdot\boldsymbol{\Gamma}^\infty+\boldsymbol{s}^{*d}\right\rangle,\left\langle-\left(\boldsymbol{H}^0\right)^{\mathrm{T}}:\boldsymbol{\Gamma}^\infty-\boldsymbol{R}^0\cdot\gamma^\infty+\boldsymbol{\phi}^{*d}\right\rangle\right)=(0,0), \tag{41}$$
$$\left\langle\boldsymbol{\Gamma}^\infty:\left(\boldsymbol{C}^0:\boldsymbol{\Gamma}^\infty+\boldsymbol{H}^0:\gamma^\infty\right)+\gamma^\infty\cdot\left(\left(\boldsymbol{H}^0\right)^{\mathrm{T}}:\boldsymbol{\Gamma}^\infty+\boldsymbol{R}^0\cdot\gamma^\infty\right)\right\rangle<0, \tag{42}$$

where $(\boldsymbol{\Gamma}^\infty,\gamma^\infty)$ are evaluated for $\left(\boldsymbol{s}^{*d},\boldsymbol{\phi}^{*d}\right)=(\boldsymbol{s}^*-\langle\boldsymbol{s}^*\rangle,\boldsymbol{\phi}^*-\langle\boldsymbol{\phi}^*\rangle)$; see Appendix A for a proof the above properties. Hence, $(\boldsymbol{\epsilon}^d,\boldsymbol{q}^d)$ can be replaced by $\left(-\boldsymbol{\Gamma}^\infty\left(\boldsymbol{s}^{*d},\boldsymbol{\phi}^{*d}\right),-\gamma^\infty\left(\boldsymbol{s}^{*d},\boldsymbol{\phi}^{*d}\right)\right)$, and the following inequality is obtained from Eq. (39):

$$\left\langle \frac{1}{2}\boldsymbol{\epsilon}^{EQ}:\boldsymbol{C}:\boldsymbol{\epsilon}^{EQ}+\boldsymbol{\epsilon}^{EQ}:\boldsymbol{H}\cdot\boldsymbol{q}^{EQ}+\frac{1}{2}\boldsymbol{q}^{EQ}\cdot\boldsymbol{R}\cdot\boldsymbol{q}^{EQ}\right\rangle<\frac{1}{2}\boldsymbol{E}:\boldsymbol{C}^0:\boldsymbol{E}+\boldsymbol{E}:\boldsymbol{H}^0\cdot\boldsymbol{Q}$$
$$+\frac{1}{2}\boldsymbol{Q}\cdot\boldsymbol{R}^0\cdot\boldsymbol{Q}-J(\boldsymbol{s}^*,\boldsymbol{\phi}^*;\boldsymbol{\Gamma}^\infty,\gamma^\infty;\boldsymbol{E},\boldsymbol{Q}).$$

The functional J in the right side is computable in terms of the Green's functions of the homogeneous infinite domain. Since the left side of Eq. (39) is replaced by the effective moduli, $(\overline{\boldsymbol{C}}^{EQ},\overline{\boldsymbol{H}}^{EQ},\overline{\boldsymbol{R}}^{EQ})$, it follows that when the RVE is subjected to the uniform boundary conditions given by Eq. (9), we have

$$\frac{1}{2}\boldsymbol{E}\colon(\overline{\boldsymbol{C}}^{EQ}-\boldsymbol{C}^0)\colon\boldsymbol{E}+\boldsymbol{E}\colon(\overline{\boldsymbol{H}}^{EQ}-\boldsymbol{H}^0)\cdot\boldsymbol{Q}+\frac{1}{2}\boldsymbol{Q}\cdot(\overline{\boldsymbol{R}}^{EQ}-\boldsymbol{R}^0)\cdot\boldsymbol{Q}<-J(\boldsymbol{s}^*,\boldsymbol{\phi}^*;\boldsymbol{\Gamma}^\infty,\gamma^\infty;\boldsymbol{E},\boldsymbol{Q}). \tag{43}$$

In essentially the same manner, Theorem I is used to produce computable bounds using the Green functions of the homogeneous infinite domain. Theorem I is written as

$$\left\langle\frac{1}{2}\boldsymbol{\sigma}^{\Sigma P}\colon\boldsymbol{D}\colon\boldsymbol{\sigma}^{\Sigma P}+\boldsymbol{\sigma}^{\Sigma P}\colon\boldsymbol{L}\cdot\boldsymbol{p}^{\Sigma P}+\frac{1}{2}\boldsymbol{p}^{\Sigma P}\cdot\boldsymbol{K}\cdot\boldsymbol{p}^{\Sigma P}\right\rangle<\left\langle\frac{1}{2}\left(\boldsymbol{\Sigma}+\boldsymbol{\sigma}^d\right)\colon\boldsymbol{D}\colon\left(\boldsymbol{\Sigma}+\boldsymbol{\sigma}^d\right)+\left(\boldsymbol{\Sigma}+\boldsymbol{\sigma}^d\right)\colon\boldsymbol{L}\cdot\left(\boldsymbol{P}+\boldsymbol{p}^d\right)+\frac{1}{2}\left(\boldsymbol{P}+\boldsymbol{p}^d\right)\cdot\boldsymbol{K}\cdot\left(\boldsymbol{P}+\boldsymbol{p}^d\right)\right\rangle, \tag{44}$$

where $(\boldsymbol{\sigma}^{\Sigma P},\boldsymbol{p}^{\Sigma P})$ are the stress field and the electric field when V is subjected to the uniform boundary data given by Eq. (10). When $\left(\boldsymbol{D}^0,\boldsymbol{L}^0,\boldsymbol{K}^0\right)$ are chosen such that $\left(\boldsymbol{D}-\boldsymbol{D}^0,\boldsymbol{L}-\boldsymbol{L}^0,\boldsymbol{K}-\boldsymbol{K}^0\right)$ are negative-definite, the right side of Eq. (44) is evaluated, as

$$\frac{1}{2}\boldsymbol{\Sigma}\colon(\overline{\boldsymbol{D}}^{\Sigma P}-\boldsymbol{D}^0)\colon\boldsymbol{\Sigma}+\boldsymbol{\Sigma}\colon(\overline{\boldsymbol{L}}^{\Sigma P}-\boldsymbol{L}^0)\cdot\boldsymbol{P}+\frac{1}{2}\boldsymbol{P}\cdot(\overline{\boldsymbol{K}}^{\Sigma P}-\boldsymbol{K}^0)\cdot\boldsymbol{P}<-I(\boldsymbol{e}^*,\boldsymbol{\psi}^*;\boldsymbol{\Lambda}^\infty,\boldsymbol{\lambda}^\infty;\boldsymbol{\Sigma},\boldsymbol{P}) \tag{45}$$

for any arbitrary $(\boldsymbol{e}^*,\boldsymbol{\psi}^*)$, where $(\overline{\boldsymbol{D}}^{\Sigma\phi},\overline{\boldsymbol{L}}^{\Sigma P},\overline{\boldsymbol{K}}^{\Sigma P})$ are the effective moduli of the RVE subjected to the uniform boundary conditions given by Eq. (10), and $(\boldsymbol{\Lambda}^\infty,\boldsymbol{\lambda}^\infty)$ are integral operators associated with $(\boldsymbol{G}^{\infty 2},\boldsymbol{g}^{\infty 2})$ and $(\boldsymbol{G}^{\infty 1},g^{\infty 1})$, satisfying the same properties as given by Eqs. (40)–(42).

It should be noted that the effective moduli $(\overline{\boldsymbol{C}}^{\Sigma P},\overline{\boldsymbol{H}}^{\Sigma P},\overline{\boldsymbol{R}}^{\Sigma P})$ which are the inverse of $(\overline{\boldsymbol{D}}^{\Sigma P},\overline{\boldsymbol{L}}^{\Sigma P},\overline{\boldsymbol{K}}^{\Sigma P})$ are almost the same as $(\overline{\boldsymbol{C}}^{EQ},\overline{\boldsymbol{H}}^{EQ},\overline{\boldsymbol{R}}^{EQ})$ when V is statistically homogeneous. Therefore, the effective moduli of the statistically homogeneous RVE are bounded by Eqs. (43) and (45). In view of Eq. (37), we finally obtain bounds for these effective moduli, denote by $\left(\overline{\boldsymbol{C}},\overline{\boldsymbol{H}},\overline{\boldsymbol{R}}\right)$, as follows: if $\left(\boldsymbol{C}^0-\boldsymbol{C},\boldsymbol{H}^0-\boldsymbol{H},\boldsymbol{R}^0-\boldsymbol{R}\right)$ is positive- (negative-) definite, then

$$\frac{1}{2}\boldsymbol{E}\colon\overline{\boldsymbol{C}}^G\colon\boldsymbol{E}+\boldsymbol{E}\colon\overline{\boldsymbol{H}}^G\cdot\boldsymbol{Q}+\frac{1}{2}\boldsymbol{Q}\cdot\overline{\boldsymbol{R}}^G\cdot\boldsymbol{Q}<(\text{or}>)-J(\boldsymbol{s}^*,\phi^*;\boldsymbol{\Gamma}^\infty,\gamma^\infty;\boldsymbol{E},\boldsymbol{Q})+\frac{1}{2}\boldsymbol{E}\colon\boldsymbol{C}^0\colon\boldsymbol{E}+\boldsymbol{E}\colon\boldsymbol{H}^0\cdot\boldsymbol{Q}+\frac{1}{2}\boldsymbol{Q}\cdot\boldsymbol{R}^0\cdot\boldsymbol{Q}. \tag{46}$$

5. Computable bounds using Green's functions of infinite body

We seek to compute the values of the bounds for the piezoelectric effective moduli which are formally given by Eqs. (43) and (45). It should be noted that the existence [11] of Eshelby-type tensors (Eshelby, 1957) can be established for the coupled piezoelectricity problems, and, indeed, general expressions are obtained for these tensors. After the existence of Eshelby's tensors for piezoelectricity is established, explicit Fourier transform expressions of these tensors are given in this section. These expressions can be numerically computed in a straightforward manner.

For simplicity, we use the following governing equations for the mechanical displacement and electric potential, $\boldsymbol{u}$ and u, instead of Eq. (27):

$$\begin{aligned}&\nabla\cdot(\boldsymbol{C}^{0\prime}\colon(\nabla\otimes\boldsymbol{u}))-\nabla\cdot(\boldsymbol{L}^{0\prime}\colon(\nabla u))+\nabla\cdot\boldsymbol{\sigma}^*=0,\\&-\nabla\cdot(\boldsymbol{K}^{0\prime}\cdot(\nabla u))-\nabla\cdot((\boldsymbol{L}^{0\prime})^{\mathrm{T}}\colon(\nabla\otimes\boldsymbol{u}))+\nabla\cdot\boldsymbol{q}^*=0.\end{aligned} \tag{47}$$

[11] Benveniste (1992) examines the existence of Eshelby's tensors for the piezoelectricity problem.

where $(\boldsymbol{\sigma}^*, \boldsymbol{q}^*)$ are eigenstress and eigen-electric displacement.

5.1. Existence of Eshelby's tensors for piezoelectricity

Consider an unbounded uniform body, B. It is assumed [12] that eigenstress and eigen-electric displacment, $(\boldsymbol{\sigma}^*, \boldsymbol{q}^*)$, are uniformly distributed within an ellipsoidal domain, Ω, contained in B.

Dunn and Wienecke (1996) have obtained the Green's function, $(\boldsymbol{G}^{\infty 2}, g^{\infty 2})$ and $(\boldsymbol{G}^{\infty 1}, g^{\infty 1})$, for the unbounded transversely isotropic body; the constitutive relations with the transverse isotropy and the x_3-axis as the axis of symmetry are

$$\begin{bmatrix} [\sigma] \\ [q] \end{bmatrix} = \begin{bmatrix} [C^{0\prime}] & [L^{0\prime}] \\ -[L^{0\prime}]^{\mathrm{T}} & [K^{0\prime}] \end{bmatrix} \begin{bmatrix} [W] & [0] \\ [0] & [1^{(3)}] \end{bmatrix} \begin{bmatrix} [\epsilon] \\ [p] \end{bmatrix}, \tag{48}$$

where $[\sigma]^{\mathrm{T}} = [\sigma_{11}, \sigma_{22}, \ldots, \sigma_{12}]$, $[q]^{\mathrm{T}} = [q_1, q_2, q_3]$, $[\epsilon]^{\mathrm{T}} = [\epsilon_{11}, \epsilon_{22}, \ldots, \epsilon_{12}]$, and $[p]^{\mathrm{T}} = [p_1, p_2, p_3]$. The matrices $[W]$ and $[1^{(3)}]$ are a diagonal matrix consisting of $(1, 1, 1, 2, 2, 2)$ and a 3×3 unit matrix; see Appendix B for explicit form of $([C^{0\prime}], [L^{0\prime}], [K^{0\prime}])$. The Green's functions are expressed in terms of the weighted distance parameters defined by

$$(R_\alpha)^2 = x_1^2 + x_2^2 + (v_\alpha x_3)^2, \tag{49}$$

for $\alpha = 0, 1, 2, 3$, where v_α's are determined from the piezoelectric moduli.

Now, we consider the second-order derivative of the Green's functions; in component form, they are

$$\frac{\partial^2 G_{ik}^{\infty 2}}{\partial x_j \partial x_l}(\boldsymbol{x} - \boldsymbol{y}), \qquad \frac{\partial^2 g_i^{\infty 2}}{\partial x_j \partial j_l}(\boldsymbol{x} - \boldsymbol{y}), \qquad \frac{\partial^2 G_k^{\infty 1}}{\partial x_j \partial x_l}(\boldsymbol{x} - \boldsymbol{y}), \qquad \frac{\partial^2 g^{\infty 1}}{\partial x_j \partial x_l}(\boldsymbol{x} - \boldsymbol{y}),$$

where $\boldsymbol{x}$ is a point at which the response is measured and $\boldsymbol{y}$ is a point at which a concentrated force or charge is applied. The derivative is expressed in terms of polyharmonic functions of R_α's. Following Walpole (1966), it is shown that the relevant integrals of the derivatives with respect to $\boldsymbol{y}$ are constants when measured at $\boldsymbol{x}$ lying within Ω. Hence, the results yield Eshelby's tensors for the piezoelectricity problem.

5.2. Expression of Eshelby's tensor for piezoelectricity

Once the existence of (constant) Eshelby's tensors for the piezoelectricity problem is established, these tensors can be computed numerically by using the Fourier transform, even though analytic expressions are not available. The required computation is straightforward. The governing equations (47) are solved by taking the Fourier transform of $\boldsymbol{u}$ and u. The associated stain and electric fields are expressed as

[12] The right sides of Eq. (47) are rewritten as $\nabla \cdot \left(\boldsymbol{C}^{0\prime} : (\nabla \otimes \boldsymbol{u})\right) + \boldsymbol{b}$ and $\nabla \cdot \left(\boldsymbol{K}^{0\prime} \cdot (\nabla u)\right) + b$, where $\boldsymbol{b} = \nabla \cdot \boldsymbol{\sigma}^* - \nabla \cdot \left(\boldsymbol{L}^{0\prime} \cdot (\nabla u)\right)$ and $\boldsymbol{b} = \nabla \cdot \boldsymbol{q}^* + \nabla \cdot ((\boldsymbol{L}^{0\prime})^{\mathrm{T}} : (\nabla \otimes \boldsymbol{u}))$ are regarded as body forces and electric charges. When $\boldsymbol{\sigma}^*$ and $\boldsymbol{q}^*$ are uniform in Ω, by definition, $\nabla \cdot \boldsymbol{\sigma}^*$ and $\nabla \cdot \boldsymbol{q}^*$ produce body forces and electric charges which behave like delta functions across the boundary $\partial\Omega$ of Ω. The remaining body forces and electric charges, $-\nabla \cdot \left(\boldsymbol{L}^{0\prime} \cdot (\nabla u)\right)$ and $\nabla \cdot ((\boldsymbol{L}^{0\prime})^{\mathrm{T}} : (\nabla \otimes \boldsymbol{u}))$, vanish in Ω, but smoothly decay outside of Ω. Therefore, Eshelby's tensors for the coupled piezoelectricity problem are different from those for the uncoupled mechanical and non-mechanical problems, even if the same ellipsoidal domain with the same (uncoupled) moduli are considered.

$$\begin{bmatrix} \boldsymbol{\epsilon}(\boldsymbol{x}) \\ \boldsymbol{p}(\boldsymbol{x}) \end{bmatrix} = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \mathrm{d}V_\xi \int_\Omega \mathrm{d}V_y \; \exp(\imath \xi \cdot (\boldsymbol{x} - \boldsymbol{y})) \times \begin{bmatrix} \mathrm{sym}^{(4)}\{\xi \otimes \boldsymbol{A}^2(\xi) \otimes \xi\} : \boldsymbol{\sigma}^*(\boldsymbol{y}) - \mathrm{sym}^{(3)}\{\xi \otimes \boldsymbol{A}^1(\xi) \otimes \xi\} \cdot \boldsymbol{q}^*(\boldsymbol{y}) \\ \left(\mathrm{sym}^{(3)}\{\xi \otimes \boldsymbol{A}^1(\xi) \otimes \xi\}\right)^{\mathrm{T}} : \boldsymbol{\sigma}^*(\boldsymbol{y}) + A^0(\xi)\{\xi \otimes \xi\} \cdot \boldsymbol{q}^*(\boldsymbol{y}) \end{bmatrix}, \tag{50}$$

where $\boldsymbol{A}^2$, $\boldsymbol{A}^1$, and A^0 are a second-order tensor, a vector, and a scalar defined by

$$\boldsymbol{A}^2(\xi) = (\tilde{\boldsymbol{C}}^{0\prime}(\xi) + \frac{1}{\tilde{K}^{0\prime}(\xi)} \xi \otimes \xi)^{-1}, \qquad \boldsymbol{A}^1(\xi) = A^0(\xi)\xi \cdot (\tilde{\boldsymbol{C}}^{0\prime}(\xi))^{-1},$$
$$A^0(\xi) = \frac{1}{\tilde{K}^{0\prime}(\xi) + \tilde{\boldsymbol{L}}^{0\prime}(\xi) \cdot (\tilde{\boldsymbol{C}}^{0\prime})^{-1}(\xi) \cdot \tilde{\boldsymbol{L}}^{0\prime}(\xi)}, \tag{51}$$

with [13] $\tilde{\boldsymbol{C}}^{0\prime} = \xi \cdot \boldsymbol{C}^{0\prime} \cdot \xi$, $\tilde{\boldsymbol{L}}^{0\prime} = \xi \cdot \boldsymbol{L}^{0\prime} \cdot \xi$, and $\tilde{K}^{0\prime} = \xi \cdot \boldsymbol{K}^{0\prime} \cdot \xi$, and, in component form, $\mathrm{sym}^{(4)}\{(.)\}_{ijkl} = ((.)_{ijkl} + (.)_{jikl} + (.)_{ijlk} + (.)_{jilk})/4$ and $\mathrm{sym}^{(3)}\{(.)\}_{ijk} = ((.)_{ijk} + (.)_{jik})/2$. These $(\boldsymbol{\epsilon}, \boldsymbol{p})$ do not depend on $\boldsymbol{x}$ when $\boldsymbol{x}$ is within Ω, i.e.,

$$(\boldsymbol{\epsilon}(\boldsymbol{x}), \boldsymbol{p}(\boldsymbol{x})) = \left(\boldsymbol{T}^4 : \boldsymbol{\sigma}^* - \boldsymbol{T}^3 \cdot \boldsymbol{q}^*, (\boldsymbol{T}^3)^{\mathrm{T}} : \boldsymbol{\sigma}^* + \boldsymbol{T}^2 \cdot \boldsymbol{q}^*\right), \tag{52}$$

for any $\boldsymbol{x}$ in Ω. Here, $(\boldsymbol{T}^4, \boldsymbol{T}^3, \boldsymbol{T}^2)$ are the fourth-, third-, and second-order Eshelby's tensors [14] for the piezoelectricity. These tensors can be computed by taking the volume average of Eq. (50) over Ω, as follows:

$$\begin{bmatrix} \boldsymbol{T}^4 \\ \boldsymbol{T}^3 \\ \boldsymbol{T}^2 \end{bmatrix}^{\mathrm{T}} = \frac{\Omega}{(2\pi)^3} \int_{-\infty}^{\infty} \mathrm{d}V_\xi \, g(\xi) g(-\xi) \begin{bmatrix} \mathrm{sym}^4\{\xi \otimes \boldsymbol{A}^2(\xi) \otimes \xi\} \\ \mathrm{sym}^3\{\xi \otimes \boldsymbol{A}^1(\xi) \otimes \xi\} \\ A^0(\xi) \xi \otimes \xi \end{bmatrix}, \tag{53}$$

where g is the g-integral [15] defined by

$$g(\xi) = \frac{1}{\Omega} \int_\Omega \exp(\imath \xi \cdot \boldsymbol{x}) \, \mathrm{d}V_x. \tag{54}$$

When the coordinates are chosen to be parallel to the three axes of the ellipsoid of the lengths a_i $(i = 1, 2, 3)$, g becomes $g = 3(\sin \eta - \eta \cos \eta)/\eta^3$ with $\eta = \sqrt{(\xi_1 a_1)^2 + (\xi_2 a_2)^2 + (\xi_3 a_3)^2)}$.

For the transversely isotropic case, $\left(\tilde{\boldsymbol{C}}^{0\prime}, \tilde{\boldsymbol{L}}^{0\prime}, \tilde{K}^{0\prime}\right)$ appearing in Eq. (51) are expressed in the following matrix form:

[13] These $\tilde{\boldsymbol{C}}^{0\prime}$, $\tilde{\boldsymbol{L}}^{0\prime}$, and $\tilde{K}^{0\prime}$ are a second-order tensor, a vector, and a scalar.

[14] Whereas Eshelby's tensor for the mechanical problem relates eigenstrain to the disturbance strain, these $(\boldsymbol{T}^4, \boldsymbol{T}^3, \boldsymbol{T}^2)$ relate eigenstress and eigen-electric displacement to the disturbance strain and electric field.

[15] See Iwakuma and Nemat-Nasser (1983), who computed g for a case of periodic structure, using the Fourier transform of the characteristic function for Ω; see also Nemat-Nasser and Hori (1993), and Mura (1987).

$$\left[\tilde{C}^{0\prime}\right] = \begin{bmatrix} C^{0\prime}_{1111}(\xi_1)^2 + C^{0\prime}_{1212}(\xi_2)^2 + C^{0\prime}_{1313}(\xi_3)^2 & \left(C^{0\prime}_{1122} - C^{0\prime}_{1212}\right)\xi_1\xi_2 & (C^{0\prime}_{1133} + C^{0\prime}_{1313})\xi_1\xi_3 \\ (C^{0\prime}_{1122} - C^{0\prime}_{1212})\xi_1\xi_2 & C^{0\prime}_{1212}(\xi_1)^2 + C^{0\prime}_{1111}(\xi_2)^2 + C^{0\prime}_{1313}(\xi_3)^2 & (C^{0\prime}_{1313} + C^{0\prime}_{1313})\xi_2\xi_3 \\ (C^{0\prime}_{1133} + C^{0\prime}_{1313})\xi_1\xi_3 & (C^{0\prime}_{1313} + C^{0\prime}_{1313})\xi_2\xi_3 & C^{0\prime}_{3333}(\xi_3)^3 \end{bmatrix}$$

$$\left[\tilde{L}^{0\prime}\right] = \begin{bmatrix} \left(L^{0\prime}_{113} + L^{0\prime}_{131}\right)\xi_1\xi_3 \\ \left(L^{0\prime}_{113} + L^{0\prime}_{131}\right)\xi_2\xi_3 \\ L^{0\prime}_{131}\left((\xi_1)^2 + (\xi_2)^2\right) + L^{0\prime}_{333}(\xi_3)^2 \end{bmatrix}, \qquad \tilde{K}^{0\prime} = K^{0\prime}_{11}\left((\xi_1)^2 + (\xi_2)^2\right) + K^{0\prime}_{33}(\xi_3)^2;$$

see Appendix B for the matrix expression of $\left(\boldsymbol{C}^{0\prime}, \boldsymbol{L}^{0\prime}, K^{0\prime}\right)$ in terms of $(C^{0\prime}_{ijkl}, L^{0\prime}_{ijk}, K^{0\prime}_{ij})$. For the transversely isotropic case, therefore, Eshelby's tensors for the piezoelectricity problem, namely, $(\boldsymbol{\Gamma}^4, \boldsymbol{\Gamma}^3, \boldsymbol{\Gamma}^2)$, can be determined by using $(\boldsymbol{A}^2, \boldsymbol{A}^1, A^0)$ which are computed from Eq. (51) with the above $\left(\tilde{\boldsymbol{C}}^{0\prime}, \tilde{\boldsymbol{L}}^{0\prime}, \tilde{K}^{0\prime}\right)$.

6. Concluding remarks

For heterogeneous piezoelectric materials, rigorous upper and lower bounds for the effective moduli are obtained by generalizing the Hashin–Shtrikman variational principle to the coupled problems of piezoelectricity. The key in deriving the bounds is the choice of the field variables, a pair of kinematics and statics eigen-quantities, i.e., $(\boldsymbol{\epsilon}^*, \boldsymbol{q}^*)$ or $(\boldsymbol{\sigma}^*, \boldsymbol{p}^*)$. The generalized Hashin–Shtrikman variational principles are formulated in essentially the same manner as the uncoupled mechanical or non-mechanical cases. Computable bounds are obtained using the Green's functions of an unbounded homogeneous body, and Eshelby's tensors for the piezoelectricity problem are determined.

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Appendix A. Properties of integral operators

The three properties of the integral operators $(\boldsymbol{\Gamma}^\infty, \boldsymbol{\gamma}^\infty)$, Eqs. (40)–(42), are proved in essentially the same manner as in the case of the uncoupled mechanical problems. As a consequence of the existence of Eshelby's tensor for the piezoelectricity problem, these operators satisfy

$$\langle \boldsymbol{\Gamma}^\infty(\boldsymbol{s}^*, \phi^*)\rangle = \boldsymbol{\Gamma}^4 : \langle \boldsymbol{s}^*\rangle + \boldsymbol{\Gamma}^3 \cdot \langle \phi^*\rangle,$$
$$\langle \boldsymbol{\gamma}^\infty(\boldsymbol{s}^*, \phi^*)\rangle = (\boldsymbol{\Gamma}^3)^{\mathrm{T}} : \langle \boldsymbol{s}^*\rangle + \boldsymbol{\Gamma}^2 \cdot \langle \phi^*\rangle,$$

for ellipsoidal V, where $\boldsymbol{\Gamma}^{4,3,2}$ are defined by Eq. (53). This yields Eqs. (40) and (41), since $(\boldsymbol{s}^{*d}, \phi^{*d})$ have zero volume average. It is easily seen from the Fourier transform of $(\boldsymbol{\Gamma}^\infty, \boldsymbol{\gamma}^\infty)$ that the integration of the following integration over a parallelepiped domain, U, vanishes as the size of the domain goes to infinity.

$$\int_U \boldsymbol{\Gamma}^\infty : \left(\boldsymbol{C}^0 : \boldsymbol{\Gamma}^\infty + \boldsymbol{H}^0 : \boldsymbol{\gamma}^\infty - \boldsymbol{s}\right) + \boldsymbol{\gamma}^\infty \cdot \left((\boldsymbol{H}^0)^{\mathrm{T}} : \boldsymbol{\Gamma}^\infty + \boldsymbol{R}^0 \cdot \boldsymbol{\gamma}^\infty\right) \mathrm{d}V = 0.$$

Since $\left(\boldsymbol{C}^0, \boldsymbol{H}^0, \boldsymbol{R}^0\right)$ satisfy

$$\boldsymbol{\Gamma}^\infty : \left(\boldsymbol{C}^0 : \boldsymbol{\Gamma}^\infty + \boldsymbol{H}^0 \cdot \gamma^\infty\right) + \gamma^\infty \cdot \left((\boldsymbol{H}^0)^{\mathrm{T}} : \boldsymbol{\Gamma}^\infty + \boldsymbol{R}^0 \cdot \gamma^\infty\right) = \boldsymbol{\Gamma}^\infty : \boldsymbol{C}^0 : \boldsymbol{\Gamma}^\infty + 2\boldsymbol{\Gamma}^\infty : \boldsymbol{H}^0 \cdot \gamma^\infty + \gamma^\infty \cdot \boldsymbol{R}^0 \cdot \gamma^\infty > 0$$

for any $(\boldsymbol{\Gamma}^\infty, \gamma^\infty)$, Eq. (42) is proved when $(\boldsymbol{s}^*, \phi^*)$ are prescribed only in Ω.

Appendix B. Transversely isotropic case

For the transversely isotropic case, the form of matrices which corresponds to $\left(\boldsymbol{C}^{0\prime}, \boldsymbol{L}^{0\prime}, \boldsymbol{K}^{0\prime}\right)$ are

$$[C^{0\prime}] = \begin{bmatrix} C^{0\prime}_{1111} & C^{0\prime}_{1111} - 2C^{0\prime}_{1212} & C^{0\prime}_{1133} & 0 & 0 & 0 \\ C^{0\prime}_{1111} - 2C^{0\prime}_{1212} & C^{0\prime}_{1111} & C^{0\prime}_{1133} & 0 & 0 & 0 \\ C^{0\prime}_{1133} & C^{0\prime}_{1133} & C^{0\prime}_{3333} & 0 & 0 & 0 \\ 0 & 0 & 0 & C^{0\prime}_{1313} & 0 & 0 \\ 0 & 0 & 0 & 0 & C^{0\prime}_{1313} & 0 \\ 0 & 0 & 0 & 0 & 0 & C^{0\prime}_{1212} \end{bmatrix},$$

$$[L^{0\prime}] = \begin{bmatrix} 0 & 0 & 0 & 0 & L^{0\prime}_{131} & 0 \\ 0 & 0 & 0 & L^{0\prime}_{131} & 9 & 0 \\ L^{0\prime}_{113} & L^{0\prime}_{113} & L^{0\prime}_{333} & 0 & 0 & 0 \end{bmatrix}, \quad [K^{0\prime}] = \begin{bmatrix} K^{0\prime}_{11} & 0 & 0 \\ 0 & K^{0\prime}_{11} & 0 \\ 0 & 0 & K^{0\prime}_{33} \end{bmatrix}.$$

References

Balendran, B., Nemat-Nasser, S., 1995. Bounds on elastic moduli of composites. J. Mech. Phys. Solids 43 (11), 1825–1853.

Benveniste, Y., 1992. The determination of the elastic and electric fields in a piezoelectric inhomogeneity. J. Appl. Phys. 72 (3), 1086–1095.

Benveniste, Y., 1997. Piezoelectric inhomogeneity problems in anti-plane shear and in-plane electric fields-how to obtain the coupled fields from the uncoupled dielectric solution. Mech. Mater. 25 (1), 59–65.

Dunn, M.L., Taya, M., 1994. Electroelastic field concentrations in and around inhomogeneities in piezoelectric solids. Trans. ASME, J. Appl. Mech. 61 (2), 474–475.

Dunn, M.L., Wienecke, H.A., 1996. Green's functions for transversely isotropic piezoelectric solids. Int. J. Solids Struct. 33 (30), 4571–4581.

Eshelby, J.D., 1957. The determination of the elastic field of an ellipsoidal inclusion, and related problems. Proc. Roy. Soc. A 241, 376–396.

Francfort, G.A., Murat, F., 1986. Homogenization and optimal bounds in linear elasticity. Arch. Rat. Mech. Anal. 94, 307–334.

Hashin, Z., Shtrikman, S., 1962. On some variational principles in anisotropic and nonhomogeneous elasticity. J. Mech. Phys. Solids 10, 335–342.

Hill, R., 1963. Elastic properties of reinforced solids: Some theoretical principles. J. Mech. Phys. Solids 11, 357–372.

Iwakuma, T., Nemat-Nasser, S., 1983. Composites with periodic microstructure. Comput. Struct. 16 (1–4), 13–19.

Kröner, E., 1977. Bounds for effective elastic moduli of disordered materials. J. Mech. Phys. Solids 25, 137–155.

Lothe, J., Barnett, D.M., 1976. Integral formation for surface waves in piezoelectric crystals: Extensive considerations. J. Appl. Phys. 47, 1799–1807.

Lothe, J., Barnett, D.M., 1977. Further development of the theory for surface waves in piezoelectric crystals. Phys. Norvegica 8 (4), 239–254.

Milton, G.W., 1990. On characterizing the set of possible effective tensors of composite: The variational method and the translation method. Comm. Pure Appl. Math. 43, 53–125.

Milton, G.W., Kohn, R., 1988. Variational bounds on the effective moduli of anisotropic composites. J. Mech. Phys. Solids 43, 63–125.

Munashinghe, H.M.S, Hori, M., Enoki, Y., 1996. Application of Hashin–Shtrikman variational principle for computing upper and lower approximate solutions of elasto-plastic problems. In: Proceedings of International Conference on Urban Eng. in Asian Cities, pp. 1–6.

Mura, T., 1987. Micromechanics of Defects in Solids. Martinus Nijhoff, Dordrecht.
Nemat-Nasser, S., Hori, M., 1993. Micromechanics: Overall Properties of Heterogeneous Materials. North-Holland, London.
Nemat-Nasser, S., Hori, M., 1995. Universal bounds for overall properties of linear and nonlinear heterogeneous solids. Trans. ASME 117, 412–422.
Torquato, S., 1991. Random heterogeneous media: Microstructure and improved bounds on effective properties. Appl. Mech. Rev. 42 (2), 37–76.
Torquato, S., 1992. Improved bounds on the effective elastic moduli of random arrays of cylinders. J. Appl. Mech. 42 (2), 37–76.
Walpole, L.J., 1966. On bounds for the overall elastic moduli of inhomogeneous systems – I. J. Mech. Phys. Solids 14, 151–162.
Willis, J.R., 1977. Bounds and self-consistent estimates for the overall properties of anisotropic composites. J. Mech. Phys. Solids 25, 185–202.