



Connection between the Conductivity and Bulk Modulus of Isotropic Composite Materials

L. V. Gibiansky, S. Torquato

Proceedings: Mathematical, Physical and Engineering Sciences, Volume 452, Issue 1945 (Feb. 8, 1996), 253-283.

Stable URL:

<http://links.jstor.org/sici?sici=1364-5021%2819960208%29452%3A1945%3C253%3ACBTCAB%3E2.0.CO%3B2-0>

Your use of the JSTOR archive indicates your acceptance of JSTOR's Terms and Conditions of Use, available at <http://www.jstor.org/about/terms.html>. JSTOR's Terms and Conditions of Use provides, in part, that unless you have obtained prior permission, you may not download an entire issue of a journal or multiple copies of articles, and you may use content in the JSTOR archive only for your personal, non-commercial use.

Each copy of any part of a JSTOR transmission must contain the same copyright notice that appears on the screen or printed page of such transmission.

Proceedings: Mathematical, Physical and Engineering Sciences is published by The Royal Society. Please contact the publisher for further permissions regarding the use of this work. Publisher contact information may be obtained at <http://www.jstor.org/journals/rsl.html>.

Proceedings: Mathematical, Physical and Engineering Sciences
©1996 The Royal Society

JSTOR and the JSTOR logo are trademarks of JSTOR, and are Registered in the U.S. Patent and Trademark Office. For more information on JSTOR contact jstor-info@umich.edu.

©2002 JSTOR

Connection between the conductivity and bulk modulus of isotropic composite materials

BY L. V. GIBIANSKY AND S. TORQUATO

*Department of Civil Engineering and Operations Research
and the Princeton Materials Institute, Princeton University,
Princeton, NJ 08544, USA*

Rigorous cross-property bounds that connect the effective electrical conductivity σ_* and the effective bulk modulus κ_* of any isotropic two-phase composite are derived when the volume fractions of the phases are either specified or unknown. These bounds enclose lens-shaped regions in the σ_* - κ_* plane, portions of which are attainable by certain microgeometries and thus are optimal. Our cross-property bounds apply also to anisotropic composites with cubic symmetry. The bounds are applied to some general situations, as well as to specific microgeometries, including regular and random arrays of spheres and hierarchical geometries corresponding to effective-medium theories. It is shown that knowledge of the effective conductivity can yield sharp estimates of the effective bulk modulus (and vice versa), even in cases where there is a wide disparity in the phase properties.

1. Introduction

The establishment of rigorous links between different effective properties of composites and other heterogeneous media, has been the subject of recent investigations (Milton 1984; Berryman & Milton 1988; Torquato 1990; Cherkaev & Gibiansky 1992, 1993; Torquato 1992; Gibiansky & Torquato 1993, 1995). Such cross-property relations are especially useful if one property of the composite is more easily measured than another physical property of the same composite. In previous papers by the authors (Gibiansky & Torquato 1993, 1995), bounds that link the effective transverse conductivity and the effective transverse elastic moduli of two-phase fibre-reinforced composites were derived. These cross-property bounds were derived using the so-called translation method, which is a powerful means of obtaining sharp bounds on effective properties. In the present paper we extend these two-dimensional results by obtaining corresponding bounds that connect the effective conductivity σ_* to the effective bulk modulus κ_* for three-dimensional two-phase isotropic or cubic symmetric composites.

Before describing our bounds we first review some previously known results. Using classical variational principles, Milton (1984) showed that, for arbitrary isotropic two-phase media, if the phase bulk moduli κ_i equal the phase conductivities σ_i and phase Poisson's ratios ν_i are positive, then the effective bulk modulus κ_* is bounded from above by the effective conductivity σ_* . It is simple to extend Milton's result to the more general situation in which $\kappa_2/\kappa_1 \leq \sigma_2/\sigma_1$ (Torquato 1992). Specifically,

for isotropic two-phase media of arbitrary topology having positive phase Poisson's ratios ν_i , the following dimensionless relation holds:

$$\kappa_*/\kappa_1 \leq \sigma_*/\sigma_1, \quad (1.1)$$

where $\kappa_2/\kappa_1 \leq \sigma_2/\sigma_1$. Corresponding results connecting the effective shear modulus to σ_* and ν_* have also been obtained.

Berryman and Milton (1988) found cross-property relations for the pairs σ_* – κ_* and σ_* – μ_* (where μ_* is the effective shear modulus) for *three-dimensional isotropic composites* by eliminating geometrical parameters involved in three-point bounds on the properties. We present their results for the conductivity–bulk modulus bounds in §7 and compare them with our results.

Our major findings are that we have obtained the sharpest known bounds on the sets of pairs σ_* – κ_* corresponding to three-dimensional two-phase isotropic composites of all possible microgeometries at a prescribed or arbitrary volume fraction f_1 by using the so-called *translation method*. These bounds enclose certain regions in the σ_* – κ_* plane. Particular boundaries of these regions (hyperbolae) are realizable by certain microgeometries and thus are optimal bounds in these instances. Our results are not restricted to isotropic composites only but apply as well to *anisotropic composites with cubic symmetry*.

We note that the determination of the electrical conductivity σ_* is mathematically equivalent to finding either the *thermal conductivity, dielectric constant, magnetic permeability or diffusion coefficient*. Thus, our cross-property relations link the elastic moduli to any of these other properties as well.

To describe the bounds, it is useful to introduce some notation. Let $F(d_1, d_2, f_1, f_2, y)$ be given by

$$F(d_1, d_2, f_1, f_2, y) = f_1 d_1 + f_2 d_2 - \frac{f_1 f_2 (d_1 - d_2)^2}{f_2 d_1 + f_1 d_2 + y}. \quad (1.2)$$

In the interest of brevity, we will further omit the first four arguments and let $F(d_1, d_2, f_1, f_2, y) = F_d(y)$.

Remark 1. This function is a scalar variant of the inverse Y -transformation. The definition and properties of the Y -transformation will be discussed in §3.

Now let σ_{1*} , σ_{2*} denote the expressions

$$\sigma_{1*} = F_\sigma(2\sigma_1), \quad \sigma_{2*} = F_\sigma(2\sigma_2), \quad (1.3)$$

$\sigma_{1\#}$, $\sigma_{2\#}$ denote the expressions

$$\sigma_{1\#} = F_\sigma(-2\sigma_1), \quad \sigma_{2\#} = F_\sigma(-2\sigma_2), \quad (1.4)$$

and κ_{1*} , κ_{2*} denote the expressions

$$\kappa_{1*} = F_\kappa\left(\frac{4}{3}\mu_1\right), \quad \kappa_{2*} = F_\kappa\left(\frac{4}{3}\mu_2\right). \quad (1.5)$$

Moreover, let σ_a and σ_h , respectively, denote the arithmetic and harmonic averages of the phase conductivities

$$\sigma_a = f_1 \sigma_1 + f_2 \sigma_2 = F_\sigma(\infty), \quad \sigma_h = \left(\frac{f_1}{\sigma_1} + \frac{f_2}{\sigma_2} \right)^{-1} = F_\sigma(0), \quad (1.6)$$

and κ_a and κ_h , respectively, denote the arithmetic and harmonic averages of the

phases bulk moduli

$$\kappa_a = f_1 \kappa_1 + f_2 \kappa_2 = F_\kappa(\infty), \quad \kappa_h = \left(\frac{f_1}{\kappa_1} + \frac{f_2}{\kappa_2} \right)^{-1} = F_\kappa(0). \quad (1.7)$$

Remark 2. The formulae (1.3) and (1.5) coincide with the the upper and lower Hashin–Shtrikman bounds on the effective conductivity (see Hashin & Shtrikman 1962) and effective bulk modulus (see Hashin & Shtrikman 1963) of isotropic composites, respectively. The formulae (1.6), (1.7) coincide with Reuss–Voigt bounds on the effective conductivity and bulk modulus. To our knowledge, relations (1.4) do not have any physical meaning.

The cross-property bounds that we have found are given by segments of hyperbolae in the σ_* – κ_* plane with asymptotes that are parallel to the axes $\sigma_* = 0$ and $\kappa_* = 0$. For this reason we mention that every such hyperbola in the x_* – y_* plane can be described by the equation

$$D(x_* - x_0)(y_* - y_0) = 1, \quad (1.8)$$

where D is some constant. It can be defined by three points that it passes through. We denote by $\text{Hyp}[(x_1, y_1), (x_2, y_2), (x_3, y_3)]$ the segment AB of such a hyperbola that passes through the points $A = (x_1, y_1)$, $B = (x_2, y_2)$ and $C = (x_3, y_3)$. It may be parametrically described in the x_* – y_* plane as follows:

$$\left. \begin{aligned} x_* &= \gamma x_1 + (1 - \gamma)x_2 - \frac{\gamma(1 - \gamma)(x_1 - x_2)^2}{(1 - \gamma)x_1 + \gamma x_2 - x_3}, \\ y_* &= \gamma y_1 + (1 - \gamma)y_2 - \frac{\gamma(1 - \gamma)(y_1 - y_2)^2}{(1 - \gamma)y_1 + \gamma y_2 - y_3}, \end{aligned} \right\} \quad (1.9)$$

where $\gamma \in [0, 1]$. Now we are ready to state our main results.

(a) Conductivity–bulk modulus bounds

Theorem 1.1. To find cross-property bounds on the set of the pairs (σ_*, κ_*) for any isotropic composite at a fixed volume fraction $f_1 = 1 - f_2$, one should inscribe in the conductivity–bulk modulus plane the following five segments of hyperbolae:

$$\begin{aligned} &\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_1, \kappa_1)], \quad \text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_2, \kappa_2)], \\ &\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_{1\#}, \kappa_h)], \quad \text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_{2\#}, \kappa_h)], \\ &\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_a, \kappa_a)]. \end{aligned}$$

The outermost pair of these curves gives us the desired bounds (see figure 1).

Remark 3. Theorem 1.1, connecting the effective conductivity to the effective bulk modulus, is not restricted to isotropic composites only, but applies to anisotropic composites with cubic symmetry as well.

Figure 1 depicts conductivity–bulk modulus bounds for the following values of the parameters:

$$\sigma_2/\sigma_1 = 20, \quad \kappa_2/\kappa_1 = 20, \quad \nu_1 = \nu_2 = 0.3, \quad f_1 = 0.2. \quad (1.10)$$

Curves 1–5 represent five segments of the hyperbolae mentioned in theorem 1.1. The

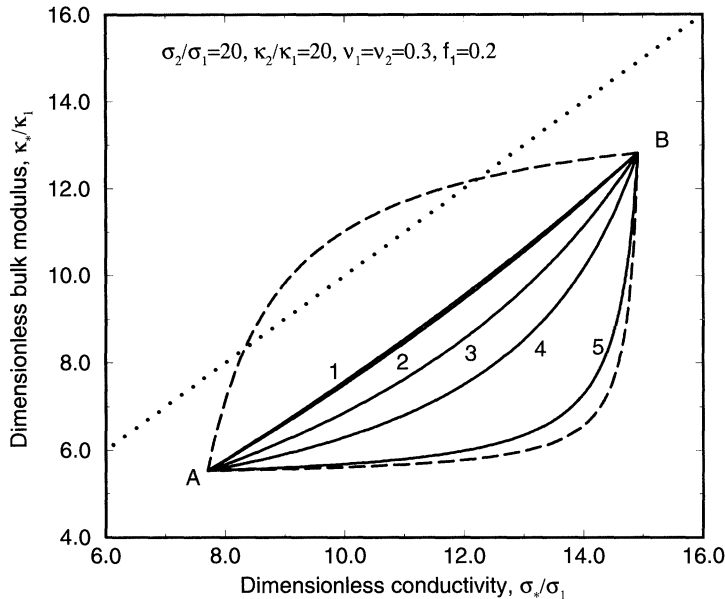


Figure 1. Cross-property bounds in the conductivity–bulk modulus plane. The internal region (bounded by curves 1 and 5) represents the bounds for fixed volume fraction. Curves 1, 2, 3, 4 and 5 are the segments of the hyperbolae described in theorem 1.1; curves 1 and 2 nearly coincide for the chosen values of the parameters. Dashed curves correspond to the Berryman–Milton bounds. The dotted line is the bound (1.1).

dashed lines correspond to the Berryman–Milton (1988) bounds (see also § 7). As can be seen, our bounds are sharper. The dotted straight line is the bound (1.1). Note that unlike the bound (1.1), our results include information about the phase volume fractions. In order to obtain bounds for arbitrary volume fraction, one can take the union of the sets defined by our bounds over the phase volume fractions (see § 5). Our results are illustrated in figure 2 for the same values of the parameters as for figure 1. The solid lines represent our bounds for fixed (shaded region) and arbitrary volume fractions. The dashed lines correspond to the Berryman–Milton bounds, and the dotted straight line again corresponds to the upper bound of relation (1.1). This bound is optimal and coincides with our new bound when $\sigma_2/\sigma_1 = \kappa_2/\kappa_1$ and the Poisson's ratios of the phases are equal to zero (i.e. $2\mu_1/3\kappa_1 = 2\mu_2/3\kappa_2 = 1$). In general, our volume-fraction independent bounds are the most restrictive.

Depending upon the values of the parameters, any two of the hyperbolae 1–5 can be the outermost pair. Since it is of interest to determine whether the outer curves are optimal, i.e. whether there exist composite structures that realize the bounds, a brief discussion concerning optimal structures is given in § 6. Here we just mention the results. The corner points $A = (\sigma_{1*}, \kappa_{1*})$, and $B = (\sigma_{2*}, \kappa_{2*})$ of the set enclosed by the bounds are *optimal* because they correspond to assemblages of coated spheres (Hashin & Shtrikman 1963) as well as to isotropic matrix laminate composites (Francfort & Murat 1987). The hyperbolae $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*})](\sigma_1, \kappa_1)$ (curve 2 of figure 1) and $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*})](\sigma_2, \kappa_2)$ (curve 1 of figure 1) correspond to the assemblages of doubly coated spheres or to doubly coated matrix laminate

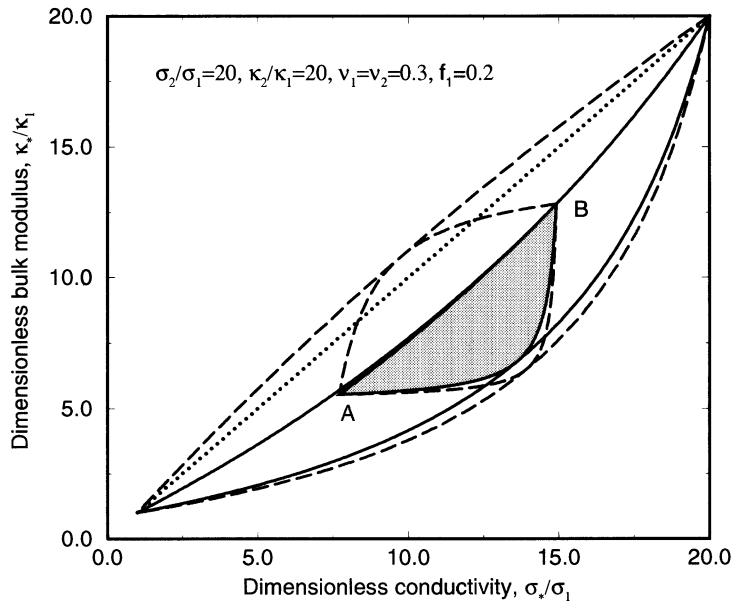


Figure 2. Cross-property bounds in the conductivity–bulk modulus plane for the composite with arbitrary and fixed volume fraction. The internal regions represent the bounds for fixed volume fraction, as depicted in figure 1, with the shaded region being our bounds. The larger external regions represent the bounds for arbitrary volume fraction. As before, solid curves show our bounds. All of the dashed curves correspond to the Berryman–Milton bounds, and the dotted line is the bound (1.1).

composites (see Schulgasser 1977; Cherkaev & Gibiansky 1992; Gibiansky & Milton 1993). Depending upon the values of the parameters, one of these curves may form part of the bound (upper bound of figure 1). Thus, this is an optimal bound because there exist composites that realize it. There are also structures that correspond to the three points on the curve $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_a, \kappa_a)]$ (curve 3 of figure 1). These are special polycrystals made of laminates of two original phases and made of coated cylinder geometries (see §6). At the moment we do not know any structures that realize the other two segments of hyperbolae $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_{1\#}, \kappa_h)]$ and $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_{2\#}, \kappa_h)]$ (curves 4 and 5 of figure 1).

In the ensuing sections we prove the bounds and apply them to a variety of different situations. Specifically, in §2 we discuss the local and homogenized equations. In §3 we describe the translation method in the context of cross-property bounds. In §§4 and 5 we use this method to prove the bounds for fixed and arbitrary volume fractions, respectively. In §6 we discuss optimal composite microstructures. In §7 we apply the bounds to a number of general cases and specific microgeometries. The reader interested only in the applications can go directly to §7.

2. Local and homogenized equations

In this section we will describe the equations that govern the electrical and elastic processes in the body and introduce a convenient system of notation that will be used to treat the problem.

The elastic state of the body is described by the local relations

$$\boldsymbol{\epsilon} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T), \quad \boldsymbol{\tau} = \mathbf{C} : \boldsymbol{\epsilon}, \quad \boldsymbol{\tau} = \boldsymbol{\tau}^T, \quad \nabla \cdot \boldsymbol{\tau} = 0, \quad (2.1)$$

where \mathbf{u} is the displacement vector, $\boldsymbol{\epsilon}$ and $\boldsymbol{\tau}$ are the strain and stress tensors, respectively, and \mathbf{C} is the stiffness tensor.

Remark 4. The symbol ‘:’ denotes contraction with regards to two indices, i.e.

$$\mathbf{a} : \mathbf{b} = \sum_{i=1}^3 \sum_{j=1}^3 a_{ij} b_{ji}, \quad \mathbf{a} = \mathbf{A} : \mathbf{b} \quad \text{if} \quad a_{ij} = \sum_{k=1}^3 \sum_{l=1}^3 A_{ijkl} b_{lk}, \quad i = 1, 2, 3, \quad j = 1, 2, 3. \quad (2.2)$$

In order to deal with the three-dimensional elasticity problem in the tensor form, we need to introduce some notations. First note that the space of the second-order tensors can be decomposed into three mutually orthogonal subspaces:

- (i) subspace Ω_h of the tensors that are proportional to identity tensor \mathbf{I} ;
- (ii) subspace Ω_s of the trace-free symmetric tensors;
- (iii) subspace Ω_a of antisymmetric tensors.

Every second-order tensor $\boldsymbol{\alpha}$ can be decomposed as follows:

$$\boldsymbol{\alpha} = \boldsymbol{\alpha}_h + \boldsymbol{\alpha}_s + \boldsymbol{\alpha}_a, \quad (2.3)$$

where

$$\boldsymbol{\alpha}_h = \frac{\text{Tr } \boldsymbol{\alpha}}{3} \mathbf{I} \in \Omega_h, \quad \boldsymbol{\alpha}_s = \frac{1}{2}(\boldsymbol{\alpha} + \boldsymbol{\alpha}^T) - \frac{\text{Tr } \boldsymbol{\alpha}}{3} \mathbf{I} \in \Omega_s, \quad \boldsymbol{\alpha}_a = \frac{1}{2}(\boldsymbol{\alpha} - \boldsymbol{\alpha}^T) \in \Omega_a. \quad (2.4)$$

Here the superscript ‘T’ in $\boldsymbol{\alpha}^T$ denotes the transpose of the tensor $\boldsymbol{\alpha}$ and $\text{Tr } \boldsymbol{\alpha} = \alpha_{11} + \alpha_{22} + \alpha_{33}$.

Let A_h , A_s , and A_a denote fourth-order tensors of projections onto the subspaces Ω_h , Ω_s and Ω_a , respectively, i.e.

$$\boldsymbol{\alpha}_h = A_h : \boldsymbol{\alpha}, \quad \boldsymbol{\alpha}_s = A_s : \boldsymbol{\alpha}, \quad \boldsymbol{\alpha}_a = A_a : \boldsymbol{\alpha}. \quad (2.5)$$

Any *isotropic* fourth-order tensor \mathbf{A} can be presented as a linear combination of these projection tensors; it can be defined by three coefficients λ_1 , λ_2 and λ_3 as follows:

$$\mathbf{A}(\lambda_1, \lambda_2, \lambda_3) = \lambda_1 A_h + \lambda_2 A_s + \lambda_3 A_a. \quad (2.6)$$

The symmetric fourth-order stiffness tensor $\mathbf{C}(3\kappa, 2\mu)$ can be written in the form (2.6) as

$$\mathbf{C}(3\kappa, 2\mu) = \mathbf{A}(3\kappa, 2\mu, 0) = 3\kappa A_h + 2\mu A_s, \quad (2.7)$$

whereas the compliance tensor is given by

$$\mathbf{S} = \mathbf{C}^{-1} = \mathbf{A}\left(\frac{1}{3\kappa}, \frac{1}{2\mu}, \infty\right). \quad (2.8)$$

Such representations reflect the fact that the stress tensor is symmetric due to the equilibrium conditions, whereas the gradient $\boldsymbol{\zeta} = \nabla \mathbf{u}$ of the displacement vector \mathbf{u} can possess a non-zero antisymmetric part.

Following Cherkaev & Gibiansky (1993), we will make use of the non-symmetric matrix $\boldsymbol{\zeta} = \nabla \mathbf{u}$ of the gradient of the displacement vector \mathbf{u} :

$$\boldsymbol{\zeta} = \nabla \mathbf{u}, \quad \boldsymbol{\zeta} = \boldsymbol{\zeta}_h + \boldsymbol{\zeta}_s + \boldsymbol{\zeta}_a. \quad (2.9)$$

Note that the projections of the tensors ζ and ϵ onto the subspaces Ω_h , Ω_s coincide, i.e.

$$\zeta_h = \epsilon_h, \quad \zeta_s = \epsilon_s, \quad (2.10)$$

and the antisymmetric part of the tensor ζ ($\zeta_a \neq \epsilon_a = 0$) does not effect the equations of elasticity. Hooke's law (2.1) can be rewritten in the form

$$\tau = \mathbf{A}(3\kappa, 2\mu, 0) : \zeta \quad (2.11)$$

or in the component form

$$\tau_h = 3\kappa\zeta_h = 3\kappa\epsilon_h, \quad \tau_s = 2\mu\zeta_s = 2\mu\epsilon_s, \quad \tau_a = 0 \cdot \zeta_a = 0. \quad (2.12)$$

We will use the following schematic matrix notation for the tensor $\mathbf{A}(\lambda_1, \lambda_2, \lambda_3)$:

$$\mathbf{A}(\lambda_1, \lambda_2, \lambda_3) = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}. \quad (2.13)$$

The isotropic stiffness and compliance tensors $\mathbf{C}(\kappa, \mu)$ and $\mathbf{S}(\kappa, \mu)$ are represented in such a form by the diagonal matrices

$$\mathbf{C}(\kappa, \mu) = \begin{pmatrix} 3\kappa & 0 & 0 \\ 0 & 2\mu & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{S}(\kappa, \mu) = \begin{pmatrix} \frac{1}{3\kappa} & 0 & 0 \\ 0 & \frac{1}{2\mu} & 0 \\ 0 & 0 & \infty \end{pmatrix}. \quad (2.14)$$

The elastic energy density can be written either as a quadratic form of strains,

$$W_\epsilon(\epsilon) = \epsilon : \mathbf{C} : \epsilon, \quad (2.15)$$

or as a quadratic form of stresses,

$$W_\tau(\tau) = \tau : \mathbf{S} : \tau. \quad (2.16)$$

The elastic energy density (2.15) as a function of the tensor ζ is given by

$$W_\epsilon(\epsilon) = W_\zeta(\zeta) = \zeta : \mathbf{C} : \zeta. \quad (2.17)$$

Henceforth, we use the following schematic notation for such forms:

$$\begin{aligned} W = \alpha : \mathbf{A}(\lambda_1, \lambda_2, \lambda_3) : \alpha &= \begin{pmatrix} \alpha_h \\ \alpha_s \\ \alpha_a \end{pmatrix}^T \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \begin{pmatrix} \alpha_h \\ \alpha_s \\ \alpha_a^T \end{pmatrix} \\ &= \lambda_1 \alpha_h : \alpha_h + \lambda_2 \alpha_s : \alpha_s + \lambda_3 \alpha_a : \alpha_a^T. \end{aligned} \quad (2.18)$$

Here λ_i are the eigenvalues of the isotropic fourth-order tensor \mathbf{A} and $\alpha = (\alpha_h \ \alpha_s \ \alpha_a)$ is a decomposition of the tensor α as a sum of projections onto three mutually orthogonal subspaces Ω_h , Ω_s and Ω_a .

The conductivity problem is described by the local relations

$$\nabla \cdot \mathbf{j} = 0, \quad \mathbf{j} = \sigma \cdot \mathbf{e}, \quad \mathbf{e} = -\nabla \phi, \quad (2.19)$$

where ψ is the electrical potential, and \mathbf{j} and \mathbf{e} are the current and electrical fields,

respectively. The tensor $\boldsymbol{\sigma}$ of the electrical conductivity of an isotropic material has the form

$$\boldsymbol{\sigma} = \sigma \mathbf{I}, \quad (2.20)$$

where σ is a conductivity constant of an isotropic media and \mathbf{I} is the (3×3) unit matrix.

The electrostatic energy density can be presented as a quadratic form in either the electric field,

$$W_e(\mathbf{e}) = \mathbf{e} \cdot \boldsymbol{\sigma} \cdot \mathbf{e}, \quad (2.21)$$

or the current field

$$W_j(\mathbf{j}) = \mathbf{j} \cdot \boldsymbol{\sigma}^{-1} \cdot \mathbf{j}. \quad (2.22)$$

It will be convenient for us to characterize the electrical properties of the material by the sum of the energies that are stored in it under the action of three mutually orthogonal electrical fields $\mathbf{e}^{(1)}$, $\mathbf{e}^{(2)}$ and $\mathbf{e}^{(3)}$:

$$W_E = W_e(\mathbf{e}^{(1)}) + W_e(\mathbf{e}^{(2)}) + W_e(\mathbf{e}^{(3)}). \quad (2.23)$$

Such a functional reflects the properties of the medium in three linear independent directions, and therefore characterizes the whole conductivity tensor of any anisotropic composite, unlike the functionals (2.21) or (2.22) that depend only on the properties of the medium in a fixed direction of the applied field. We may treat this sum as a quadratic form of the matrix $\mathbf{E} = (\mathbf{e}^{(1)} \quad \mathbf{e}^{(2)} \quad \mathbf{e}^{(3)})$:

$$W_E(\mathbf{E}) = \begin{pmatrix} \mathbf{e}^{(1)} \\ \mathbf{e}^{(2)} \\ \mathbf{e}^{(3)} \end{pmatrix}^T \begin{pmatrix} \boldsymbol{\sigma} & 0 & 0 \\ 0 & \boldsymbol{\sigma} & 0 \\ 0 & 0 & \boldsymbol{\sigma} \end{pmatrix} \begin{pmatrix} \mathbf{e}^{(1)} \\ \mathbf{e}^{(2)} \\ \mathbf{e}^{(3)} \end{pmatrix}. \quad (2.24)$$

It is convenient to use the representation of this matrix in the basis similar to the one that we used in the elasticity problem, namely, in any fixed basis \mathbf{i} , \mathbf{j} , \mathbf{k} , we can treat the triple $\mathbf{E} = (\mathbf{e}^{(1)} \quad \mathbf{e}^{(2)} \quad \mathbf{e}^{(3)})$ as a (3×3) matrix

$$\mathbf{E} = (\mathbf{e}^{(1)} \quad \mathbf{e}^{(2)} \quad \mathbf{e}^{(3)}) = \begin{pmatrix} e_1^{(1)} & e_1^{(2)} & e_1^{(3)} \\ e_2^{(1)} & e_2^{(2)} & e_2^{(3)} \\ e_3^{(1)} & e_3^{(2)} & e_3^{(3)} \end{pmatrix}. \quad (2.25)$$

The quadratic form (2.24) for an isotropic tensor $\boldsymbol{\sigma}$ can be schematically written as

$$W_E(\mathbf{E}) = \mathbf{E} \cdot \hat{\boldsymbol{\sigma}} \cdot \mathbf{E} = \begin{pmatrix} \mathbf{E}_h \\ \mathbf{E}_s \\ \mathbf{E}_a \end{pmatrix}^T \begin{pmatrix} \sigma & 0 & 0 \\ 0 & \sigma & 0 \\ 0 & 0 & \sigma \end{pmatrix} \begin{pmatrix} \mathbf{E}_h \\ \mathbf{E}_s \\ \mathbf{E}_a^T \end{pmatrix}, \quad (2.26)$$

where \mathbf{E}_h , \mathbf{E}_s and \mathbf{E}_a are the projections of the matrix \mathbf{E} onto the subspaces Ω_h , Ω_s and Ω_a , respectively, and $\hat{\boldsymbol{\sigma}} = \mathbf{A}(\sigma, \sigma, \sigma)$.

Similarly, the sum of the energies stored by conducting material in current fields $\mathbf{j}^{(1)}$, $\mathbf{j}^{(2)}$ and $\mathbf{j}^{(3)}$ can be presented as a quadratic form

$$W_J = \mathbf{J} \cdot \hat{\boldsymbol{\sigma}}^{-1} \cdot \mathbf{J} = \begin{pmatrix} \mathbf{J}_h \\ \mathbf{J}_s \\ \mathbf{J}_a \end{pmatrix}^T \begin{pmatrix} \sigma^{-1} & 0 & 0 \\ 0 & \sigma^{-1} & 0 \\ 0 & 0 & \sigma^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{J}_h \\ \mathbf{J}_s \\ \mathbf{J}_a^T \end{pmatrix}, \quad (2.27)$$

where $\mathbf{J} = (\mathbf{j}^{(1)} \quad \mathbf{j}^{(2)} \quad \mathbf{j}^{(3)})$.

(a) Homogenization

Let us consider a composite that is a space-periodic structure. The element of periodicity V is divided into two parts V_1 and V_2 with volume fractions f_1 and $f_2 = 1 - f_1$, respectively. Let us assume that these two parts are occupied by two isotropic materials with the elastic moduli (κ_1, μ_1) and (κ_2, μ_2) , and with the electrical conductivities σ_1 and σ_2 . It is desired to study the homogenization problem, i.e. the problem of describing the medium's effective properties. It is well known that the average behaviour of a mixture is described by the homogenized equations of elasticity,

$$\langle \epsilon \rangle = \frac{1}{2}(\nabla \langle u \rangle + (\nabla \langle u \rangle)^T), \quad \langle \tau \rangle = C_* : \langle \epsilon \rangle, \quad \langle \tau \rangle = \langle \tau \rangle^T, \quad \nabla \cdot \langle \tau \rangle = 0, \quad (2.28)$$

and of conductivity,

$$\langle e \rangle = -\nabla \langle \phi \rangle, \quad \langle j \rangle = \sigma_* \cdot \langle e \rangle, \quad \nabla \cdot \langle j \rangle = 0. \quad (2.29)$$

Here the symbol $\langle \cdot \rangle$ denotes averaging over the element of periodicity V , i.e.

$$\langle (\cdot) \rangle = \frac{1}{\text{vol } V} \int_V (\cdot) dV. \quad (2.30)$$

The tensor C_* , connecting the average stress and average strain, is by definition the *effective stiffness tensor*, and the tensor σ_* , connecting the average current and average electrical field, is the *effective conductivity tensor*. The effective property tensors C_* and σ_* depend on the phase properties, phase volume fraction f_1 , and the geometrical structure of the composite, independent of the loading.

Remark 5. Note that any homogeneous composite is equivalent, with respect to the effective elasticity and conductivity tensors, to some periodic structure. The assumption of periodicity is not very restrictive; it is imposed only for the sake of simplicity of description.

The elastic energy density W^* stored in the composite is known to be equal to

$$W_\epsilon^*(\epsilon_0) = \epsilon_0 : C_* : \epsilon_0 = \inf_{\substack{\langle \epsilon \rangle = \epsilon_0 \\ \epsilon = \frac{1}{2}(\nabla u + (\nabla u)^T)}} \langle \epsilon : C : \epsilon \rangle, \quad (2.31)$$

where infimum is taken over fields $\epsilon = \frac{1}{2}(\nabla u + (\nabla u)^T)$ with given mean value ϵ_0 (Beran 1968). For the conjugate functional of the complementary energy (Beran 1968), we have

$$W_\tau^*(\tau_0) = \tau_0 : S_* : \tau_0 = \inf_{\substack{\langle \tau \rangle = \tau_0 \\ \tau = \tau^T, \nabla \cdot \tau = 0}} \langle \tau : S : \tau \rangle, \quad (2.32)$$

where the effective compliance tensor S_* is determined as $S_* = C_*^{-1}$ and infimum is taken over stress fields with given mean value τ_0 that satisfy equilibrium conditions $\tau = \tau^T, \nabla \cdot \tau = 0$.

The electrostatic energy density of the composite is known to be a quadratic form in the electrical field, i.e.

$$W_e^*(e_0) = e_0 \cdot \sigma_* \cdot e_0 = \inf_{\substack{\langle e \rangle = e_0 \\ e = -\nabla \phi}} \langle e \cdot \sigma \cdot e \rangle, \quad (2.33)$$

(Dirichlet variational principle, see Beran 1968) or the current field,

$$W_j^*(j_0) = j_0 \cdot \sigma_*^{-1} \cdot j_0 = \inf_{\substack{\langle j \rangle = j_0 \\ \nabla \cdot j = 0}} \langle j \cdot \sigma^{-1} \cdot j \rangle \quad (2.34)$$

(Thomson variational principle, see Beran 1968). For the conductivity problem we use the functionals that are the sums of the energies stored by the composite in three trial fields, like (2.33) and (2.34), namely,

$$W_E^*(\mathbf{E}_0) = \mathbf{E}_0 \cdot \hat{\boldsymbol{\sigma}}_* \cdot \mathbf{E}_0 = \inf_{\substack{\langle \mathbf{E} \rangle = \mathbf{E}_0 \\ \mathbf{E} = -\nabla(\phi^{(1)}, \phi^{(2)}, \phi^{(3)})}} \langle \mathbf{E} \cdot \hat{\boldsymbol{\sigma}} \cdot \mathbf{E} \rangle \quad (2.35)$$

and

$$W_J^*(\mathbf{J}_0) = \mathbf{J}_0 \cdot \hat{\boldsymbol{\sigma}}_*^{-1} \cdot \mathbf{J}_0 = \inf_{\substack{\langle \mathbf{J} \rangle = \mathbf{J}_0 \\ \nabla \cdot \mathbf{J} = 0}} \langle \mathbf{J} \cdot \hat{\boldsymbol{\sigma}}^{-1} \cdot \mathbf{J} \rangle, \quad (2.36)$$

where the tensor $\hat{\boldsymbol{\sigma}}_*$ is defined similarly to (2.26).

3. The translation method

To prove our cross-property bounds we will use the translation method that was introduced independently by Lurie & Cherkav (1984), (1986), Murat & Tartar (1985) and Tartar (1985). The method is based on bounding from below the relevant energy functional I . We have already used the translation method to obtain conductivity–elastic moduli bounds (Gibiansky & Torquato 1995) in the corresponding two-dimensional problem. Since the derivation is similar to the two-dimensional case (although not exactly the same), we shall briefly sketch the main ideas behind the use of the translation method to obtain cross-property bounds in three dimensions. More detailed discussion and references can be found in our paper concerning the two-dimensional problem.

As in the two-dimensional problem, the following functionals should be considered for the conductivity–bulk modulus bounds:

$$I_{\zeta E}(\boldsymbol{\zeta}_h, \mathbf{E}_h) = W_{\zeta}^*(\boldsymbol{\zeta}_h) + W_E^*(\mathbf{E}_h), \quad (3.1)$$

$$I_{\zeta J}(\boldsymbol{\zeta}_h, \mathbf{J}_h) = W_{\zeta}^*(\boldsymbol{\zeta}_h) + W_J^*(\mathbf{J}_h), \quad (3.2)$$

$$I_{\tau E}(\boldsymbol{\tau}_h, \mathbf{E}_h) = W_{\tau}^*(\boldsymbol{\tau}_h) + W_E^*(\mathbf{E}_h), \quad (3.3)$$

$$I_{\tau J}(\boldsymbol{\tau}_h, \mathbf{J}_h) = W_{\tau}^*(\boldsymbol{\tau}_h) + W_J^*(\mathbf{J}_h). \quad (3.4)$$

The lower bound of each of these functionals gives some component of the boundary.

Each of the functionals described in (3.1)–(3.4) is a quadratic form of the elastic and electrical fields and can be represented in the form

$$I = \boldsymbol{\alpha}_0 \cdot \mathbf{D}_* \cdot \boldsymbol{\alpha}_0 = \inf_{\substack{\langle \boldsymbol{\alpha} \rangle = \boldsymbol{\alpha}_0 \\ \boldsymbol{\alpha} \in EK}} \langle \boldsymbol{\alpha} \cdot \mathbf{D}(\mathbf{x}) \cdot \boldsymbol{\alpha} \rangle, \quad (3.5)$$

where infimum is taken over fields $\boldsymbol{\alpha}$ with given mean value $\boldsymbol{\alpha}_0$ such that

$$\boldsymbol{\alpha} \in EK. \quad (3.6)$$

Here $\boldsymbol{\alpha}$ is a vector composed of the coefficients of tensors of gradients $\boldsymbol{\zeta}$ or stresses $\boldsymbol{\tau}$ and matrices \mathbf{E} or \mathbf{J} . The set EK is a set of space-periodic vectors that satisfy some differential restrictions. For the components of a stress tensor, these restrictions are given by the equilibrium equations $\nabla \cdot \boldsymbol{\tau} = 0$. For gradients one has $\boldsymbol{\zeta} = \nabla \mathbf{u}$. For the matrix $\mathbf{E} = -\nabla(\phi_1, \phi_2, \phi_3)$ of the electrical fields, these restrictions guarantee the potential character of these fields, and for the triple of current fields \mathbf{J} they are given

by the conditions $\nabla \cdot \mathbf{J} = 0$. The matrix \mathbf{D} is a piecewise constant block diagonal matrix composed of the coefficients of the material tensors in the form (2.13).

Let us assume that we are given so-called *quasi-convex* [*quasi-affine*] (see, for example, Dacorogna (1982) and references therein) quadratic functions of the fields $\boldsymbol{\alpha}$,

$$\phi(\boldsymbol{\alpha}) = \boldsymbol{\alpha} \cdot \mathbf{T} \cdot \boldsymbol{\alpha}, \quad (3.7)$$

possessing the property of convex [affine] functions

$$\langle \phi(\boldsymbol{\alpha}) \rangle \geq \phi(\langle \boldsymbol{\alpha} \rangle), \quad [\langle \phi(\boldsymbol{\alpha}) \rangle = \phi(\langle \boldsymbol{\alpha} \rangle)] \quad (3.8)$$

for every field $\boldsymbol{\alpha} \in EK$. Here \mathbf{T} is the so-called translation matrix, which is a constant matrix. Given such functions, one can prove the bound

$$\mathbf{Y}(\mathbf{D}_*) + \mathbf{T} \geq 0, \quad (3.9)$$

which is true for any matrix \mathbf{T} of a quasi-convex quadratic form such that

$$\mathbf{D}_1 - \mathbf{T} \geq 0, \quad \mathbf{D}_2 - \mathbf{T} \geq 0. \quad (3.10)$$

Here $\mathbf{Y}(\mathbf{D}_*)$ is a Y -transformation of the effective properties tensor \mathbf{D}_* ,

$$\begin{aligned} \mathbf{Y}(\mathbf{D}_1, \mathbf{D}_2, f_1, f_2, \mathbf{D}_*) \\ = -f_2 \mathbf{D}_1 - f_1 \mathbf{D}_2 - f_1 f_2 (\mathbf{D}_1 - \mathbf{D}_2) \cdot (\mathbf{D}_* - f_1 \mathbf{D}_1 - f_2 \mathbf{D}_2)^{-1} \cdot (\mathbf{D}_1 - \mathbf{D}_2), \end{aligned} \quad (3.11)$$

that was introduced by Milton (1991) and Cherkaev & Gibiansky (1992). Henceforth, we will omit the first four arguments of the Y -transformation and will denote it simply as $\mathbf{Y}(\mathbf{D}_*)$. Note that the bounds in the form (3.9) in terms of the Y -transformations do not depend on volume fractions. All the information about the volume fractions is ‘hidden’ in the definition of the Y -transformation.

Remark 6. We will use some of the properties of this transformation, namely

$$\begin{aligned} \mathbf{Y}(\mathbf{D}_1, \mathbf{D}_2, f_1, f_2, \mathbf{D}_i) &= -\mathbf{D}_i, \quad i = 1, 2, \\ \mathbf{Y}(\mathbf{D}_1^{-1}, \mathbf{D}_2^{-1}, f_1, f_2, \mathbf{D}_*^{-1}) &= \mathbf{Y}^{-1}(\mathbf{D}_1, \mathbf{D}_2, f_1, f_2, \mathbf{D}_*). \end{aligned} \quad (3.12)$$

If the matrix $(\mathbf{D}_1 - \mathbf{D}_2)$ is not degenerate then the inverse Y -transformation

$$\mathbf{D}_* = f_1 \mathbf{D}_1 + f_2 \mathbf{D}_2 - f_1 f_2 (\mathbf{D}_1 - \mathbf{D}_2) \cdot (f_1 \mathbf{D}_2 + f_2 \mathbf{D}_1 + \mathbf{D}_*)^{-1} \cdot (\mathbf{D}_1 - \mathbf{D}_2) \quad (3.13)$$

is not degenerate and the bound (3.9) leads to the bound on the tensor \mathbf{D}_* . In the problem under study, the matrix $\mathbf{D}_1 - \mathbf{D}_2$ may be degenerate, i.e. some of the eigenvectors and eigenvalues of the matrices \mathbf{D}_1 and \mathbf{D}_2 may coincide. Indeed, for any material, the stiffness matrix \mathbf{C} has one of the eigenvalues equal to zero (see (2.14)). The matrix \mathbf{C} is in turn the diagonal block of matrices \mathbf{D} used in the functionals (3.1)–(3.2). One can find the appropriate form of the bounds (3.9) for this case as well (Cherkaev & Gibiansky 1993), but here we will not go into details. As we will see, in our problem all of the matrices in matrix inequality (3.9) are block-diagonal if the component materials and the composite are isotropic, which is the case. For the block of this matrix that gives the bounds, the difference $\mathbf{D}_1 - \mathbf{D}_2$ is not degenerate and we can use the bound in the form (3.9). More exactly, we use the scalar corollary of matrix inequality (3.9), namely,

$$\det[\mathbf{Y}(\mathbf{D}_*) + \mathbf{T}] \geq 0. \quad (3.14)$$

The symmetric matrix \mathbf{T} should be chosen in order to make the bounds (3.14) the most restrictive.

(a) *Quasi-convex functions*

Let us now describe the quasi-convex functions that we need in order to prove the bounds of theorem 1.1.

Lemma 3.1.(i) *Quadratic function*

$$\phi_{JJ}(\mathbf{J}, \mathbf{J}, t_1) = \mathbf{J}^T : \mathbf{A}(-t_1, 2t_1, 0) : \mathbf{J} \quad (3.15)$$

is quasi-convex for any positive value of the parameter t_1 if matrix \mathbf{J} is divergence-free, i.e. $\nabla \cdot \mathbf{J} = 0$.

(ii) *Bilinear functions*

$$\phi_{\zeta E}(\zeta, \mathbf{E}, t_2) = \zeta^T : \mathbf{A}(-2t_2, t_2, -t_2) : \mathbf{E} \quad (3.16)$$

and

$$\phi_{\zeta J}(\zeta, \mathbf{J}, t_3) = \zeta^T : \mathbf{A}(t_3, t_3, t_3) : \mathbf{J} \quad (3.17)$$

are quasi-affine for any values of the parameters t_2 and t_3 if matrices ζ and \mathbf{E} are the gradients, i.e. $\zeta = \nabla \mathbf{u}$, $\mathbf{E} = -\nabla(\phi_1, \phi_2, \phi_3)$ and \mathbf{J} is a divergence free ($\nabla \cdot \mathbf{J} = 0$).

Remark 7. Although tensor ζ is a gradient of the displacement vector, whereas tensor \mathbf{E} is a gradient of the triple of scalar potentials, it makes no difference here, we treat them identically. The same is true for the tensors \mathbf{J} and τ . Although \mathbf{J} is an arbitrary matrix of three current fields but τ is a symmetric tensor, the function (3.15) is also quasi-convex if we substitute τ instead of \mathbf{J} . In expression (3.17), tensor \mathbf{J} can be replaced by τ and (or) tensor \mathbf{E} can be replaced by ζ preserving the quasi-convexity properties.

Proof of the lemma. We have to prove that

$$\langle \mathbf{J}^T : \mathbf{A}(-t_1, 2t_1, 0) : \mathbf{J} \rangle - \mathbf{J}_0^T : \mathbf{A}(-t_1, 2t_1, 0) : \mathbf{J}_0 \geq 0, \quad (3.18)$$

$$\langle \zeta^T : \mathbf{A}(-2t_2, t_2, -t_2) : \mathbf{E} \rangle - \zeta_0^T : \mathbf{A}(-2t_2, t_2, -t_2) : \mathbf{E}_0 = 0 \quad (3.19)$$

and

$$\langle \zeta^T : \mathbf{A}(t_3, t_3, t_3) : \mathbf{J} \rangle - \zeta_0^T : \mathbf{A}(t_3, t_3, t_3) : \mathbf{J}_0 = 0, \quad (3.20)$$

for any values of the parameters $t_1 \geq 0$, t_2 and t_3 , where \mathbf{J}_0 , ζ_0 and \mathbf{E}_0 are the average values of the correspondent fields. In order to prove it we use the Fourier decomposition of the fields and Plancherel's equality. One can check that the expressions (3.18)–(3.20) are equal, respectively, to

$$\sum_{\mathbf{k} \neq 0} \hat{\mathbf{J}}^T(\mathbf{k}) : \mathbf{A}(-t_1, 2t_1, 0) : \hat{\mathbf{J}}(\mathbf{k}), \quad (3.21)$$

$$\sum_{\mathbf{k} \neq 0} \hat{\zeta}^T(\mathbf{k}) : \mathbf{A}(-2t_2, t_2, -t_2) : \hat{\mathbf{E}}(\mathbf{k}), \quad (3.22)$$

and

$$\sum_{\mathbf{k} \neq 0} \hat{\zeta}^T(\mathbf{k}) : \mathbf{A}(t_3, t_3, t_3) : \hat{\mathbf{E}}(\mathbf{k}), \quad (3.23)$$

where \mathbf{k} is a Fourier wavevector and $\hat{\mathbf{J}}(\mathbf{k})$, $\hat{\zeta}(\mathbf{k})$ and $\hat{\mathbf{E}}(\mathbf{k})$ are Fourier coefficients of the fields \mathbf{J} , ζ and \mathbf{E} , respectively. Let us now rewrite the differential restrictions

$$\nabla \cdot \mathbf{J} = 0, \quad \zeta = \nabla \mathbf{u}, \quad \mathbf{E} = -\nabla(\phi_1, \phi_2, \phi_3) \quad (3.24)$$

for the fields \mathbf{J} , $\boldsymbol{\zeta}$ and \mathbf{E} in a Fourier space as

$$\mathbf{k} \cdot \hat{\mathbf{J}}(\mathbf{k}) = 0, \quad \hat{\boldsymbol{\zeta}}(\mathbf{k}) = \mathbf{k} \hat{\mathbf{u}}(\mathbf{k}), \quad \hat{\mathbf{E}}(\mathbf{k}) = -\mathbf{k}(\hat{\phi}_1(\mathbf{k}), \hat{\phi}_2(\mathbf{k}), \hat{\phi}_3(\mathbf{k})). \quad (3.25)$$

As follows from (3.25), for any $\mathbf{k} \neq 0$ the matrices $\hat{\mathbf{J}}(\mathbf{k})$, $\hat{\boldsymbol{\zeta}}(\mathbf{k})$ and $\hat{\mathbf{E}}(\mathbf{k})$ can be presented in the form

$$\hat{\mathbf{J}}(\mathbf{k}) = \begin{pmatrix} 0 & 0 & 0 \\ \hat{J}_{21}(\mathbf{k}) & \hat{J}_{22}(\mathbf{k}) & \hat{J}_{23}(\mathbf{k}) \\ \hat{J}_{31}(\mathbf{k}) & \hat{J}_{32}(\mathbf{k}) & \hat{J}_{33}(\mathbf{k}) \end{pmatrix}, \quad \hat{\boldsymbol{\zeta}}(\mathbf{k}) = \begin{pmatrix} \hat{\zeta}_{11}(\mathbf{k}) & \hat{\zeta}_{12}(\mathbf{k}) & \hat{\zeta}_{13}(\mathbf{k}) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (3.26)$$

$$\hat{\mathbf{E}}(\mathbf{k}) = \begin{pmatrix} \hat{E}_{11}(\mathbf{k}) & \hat{E}_{12}(\mathbf{k}) & \hat{E}_{13}(\mathbf{k}) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (3.27)$$

in the basis $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$, where the first of the basis vectors is parallel to the Fourier vector \mathbf{k} .

By substituting relations (3.26)–(3.27) into the relations (3.21)–(3.23), we arrive at (3.18)–(3.20), which completes the proof of the quasi-convexity properties (3.15)–(3.17).

4. Coupled conductivity–bulk modulus bounds

We now prove theorem 1.1 of § 1. Although the final results do not depend on the values of the parameters, the choice of the functionals that we need to study differs depending on whether

$$(\sigma_1 - \sigma_2)(\mu_1 - \mu_2) \geq 0 \quad (4.1)$$

or

$$(\sigma_1 - \sigma_2)(\mu_1 - \mu_2) \leq 0. \quad (4.2)$$

We call the pair of materials that satisfy (4.1) ‘well-ordered materials’, in contrast to ‘badly ordered materials’ that satisfy (4.2). These definitions should not be confused with the commonly used ones that involve the bulk and shear moduli.

(a) *Bulk modulus–conductivity bounds for a composite of two badly ordered materials*

(i) *Lower bounds in terms of the Y-transformation of the effective moduli*

We begin by proving the bounds in terms of the Y-transformations of the effective moduli for a composite of two badly ordered phases. Let us consider the functional $I_{\zeta E}$. It can be written as the quadratic form

$$I_{\zeta E} = \boldsymbol{\alpha}_0 \cdot \mathbf{D}_*^{\zeta E} \cdot \boldsymbol{\alpha}_0 \quad (4.3)$$

associated with the matrix

$$\mathbf{D}_*^{\zeta E} = \begin{pmatrix} \mathbf{A}(3\kappa_*, 2\mu_*, 0) & 0 \\ 0 & \mathbf{A}(\sigma_*, \sigma_*, \sigma_*) \end{pmatrix} = \begin{pmatrix} 3\kappa_* & 0 & 0 & 0 & 0 & 0 \\ 0 & 2\mu_* & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sigma_* & 0 & 0 \\ 0 & 0 & 0 & 0 & \sigma_* & 0 \\ 0 & 0 & 0 & 0 & 0 & \sigma_* \end{pmatrix} \quad (4.4)$$

and the vector

$$\boldsymbol{\alpha}_0 = \begin{pmatrix} \zeta_h & \zeta_s & \zeta_a & \mathbf{E}_h & \mathbf{E}_s & \mathbf{E}_a \end{pmatrix}. \quad (4.5)$$

As follows from (3.16), the matrix

$$\mathbf{T}^{\zeta E} = \begin{pmatrix} \mathbf{A}(-2t_1, t_1, -t_1) & \mathbf{A}(-2t_3, t_3, -t_3) \\ \mathbf{A}(-2t_3, t_3, -t_3) & \mathbf{A}(-2t_2, t_2, -t_2) \end{pmatrix} = \begin{pmatrix} -2t_1 & 0 & 0 & -2t_3 & 0 & 0 \\ 0 & t_1 & 0 & 0 & t_3 & 0 \\ 0 & 0 & -t_1 & 0 & 0 & -t_3 \\ -2t_3 & 0 & 0 & -2t_2 & 0 & 0 \\ 0 & t_3 & 0 & 0 & t_2 & 0 \\ 0 & 0 & -t_3 & 0 & 0 & -t_2 \end{pmatrix} \quad (4.6)$$

is associated with the quasi-affine quadratic form of the pair of tensors $\boldsymbol{\zeta}$ and \mathbf{E} . Restrictions for the parameters t_1 , t_2 and t_3 come from the inequality

$$\mathbf{D}_i^{\zeta E} - \mathbf{T}^{\zeta E} \geq 0, \quad i = 1, 2, \quad (4.7)$$

where $\mathbf{D}_i^{\zeta E}$, $i = 1, 2$ are the matrices of the phase properties defined similar to (4.4). The last matrix has a block-diagonal form

$$\mathbf{D}_i^{\zeta E} - \mathbf{T}^{\zeta E} = \mathbf{D}_i^{1,4} \oplus \mathbf{D}_i^{2,5} \oplus \mathbf{D}_i^{3,6}, \quad (4.8)$$

where $\mathbf{D}_i^{k,l}$ is a submatrix of the matrix $\mathbf{D}_i^{\zeta E} - \mathbf{T}^{\zeta E}$ that is composed of the elements that are the intersections of the columns with numbers k and l and rows with the same numbers. Conditions

$$\det \mathbf{D}_i^{1,4} = (3\kappa_i + 2t_1)(\sigma_i + 2t_2) - 4t_3^2 \geq 0, \quad i = 1, 2, \quad (4.9)$$

$$\det \mathbf{D}_i^{2,5} = (2\mu_i - t_1)(\sigma_i - t_2) - t_3^2 \geq 0 \quad i = 1, 2, \quad (4.10)$$

and

$$\det \mathbf{D}_i^{3,6} = t_1(\sigma_i + t_2) - t_3^2 \geq 0, \quad i = 1, 2, \quad (4.11)$$

are equivalent to (4.7). The bounds come from the inequality

$$\det[\mathbf{Y}(\mathbf{D}^{\zeta E})_* + \mathbf{T}^{\zeta E}]^{1,4} = (3y(\kappa_*) - 2t_1)(y(\sigma_*) - 2t_2) - 4t_3^2 \geq 0, \quad (4.12)$$

where $y(\sigma_*)$ and $y(\kappa_*)$ are the scalar Y -transformations of the effective conductivity and bulk modulus, respectively, i.e.

$$y(\sigma_*) = -f_2\sigma_1 - f_1\sigma_2 - \frac{f_1f_2(\sigma_1 - \sigma_2)^2}{\sigma_* - f_1\sigma_1 - f_2\sigma_2} \quad (4.13)$$

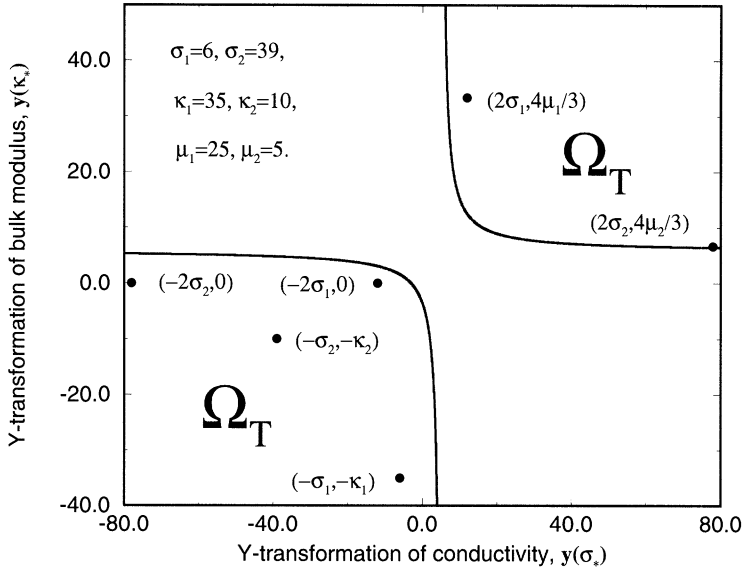


Figure 3. The set Ω_T in the $y(\sigma_*)$ – $y(\kappa_*)$ plane. This set contains the indicated points as described in the text.

and

$$y(\kappa_*) = -f_2\kappa_1 - f_1\kappa_2 - \frac{f_1f_2(\kappa_1 - \kappa_2)^2}{\kappa_* - f_1\kappa_1 - f_2\kappa_2}. \quad (4.14)$$

Let us denote as Ω_T the set of the pairs $(y(\sigma_*), y(\kappa_*))$ that satisfy inequality (4.12) for the fixed values of the parameters t_1, t_2 and t_3 (see figure 3). The bound of this set is a hyperbola in the plane σ_* – κ_* that can be written in a form (1.8) with a positive coefficient in front of the main (bilinear) term. Parameters t_1, t_2, t_3^2 uniquely define the position of the hyperbola (4.12). Therefore, moving and resizing of the set Ω_T is equivalent to varying the parameters t_1, t_2, t_3^2 . But these parameters are subject to the restrictions (4.9)–(4.11). Conditions (4.9) mean that the pairs $(-\sigma_i, -\kappa_i)$ $i = 1, 2$ belong to the set Ω_T , inequalities (4.10) require that the pairs $(2\sigma_i, 4\mu_i/3)$ lie within the set Ω_T , and conditions (4.11) are equivalent to saying that the pairs $(-2\sigma_i, 0)$ belong to Ω_T . These are the only restrictions on the parameters, and therefore on the position of the boundary hyperbola of the set Ω_T .

Analysis of the bounds (4.12) and restrictions (4.9)–(4.11) for any composite with badly ordered phases leads to the following bounds:

Theorem 4.1. *The lower bound on the set of pairs $(y(\sigma_*), y(\kappa_*))$ in the plane $y(\sigma_*)$ – $y(\kappa_*)$ is given by the lowest of the four hyperbolae*

$$\begin{aligned} &\text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-2\sigma_1, 0)], & \text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-2\sigma_2, 0)], \\ &\text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_1, -\kappa_1)], & \text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_2, -\kappa_2)]. \end{aligned}$$

We have proved the lower bound in terms of Y -transformations of the moduli.

Remark 8. Condition (4.3) guarantees the existence of the parameters t_1, t_2, t_3 such that the bounding hyperbola with the positive coefficient in front of the bilinear

term passes through the points $(2\sigma_1, \frac{4}{3}\mu_1)$, $(2\sigma_2, \frac{4}{3}\mu_2)$, simultaneously. In this case, the conditions (4.10), $i = 1, 2$, are equalities and define two equations for the three parameters t_1, t_2, t_3 . The strongest one among conditions (4.9), (4.11), $i = 1, 2$ defines the third equality that allows one to find all of the coefficients. One can analyse these conditions (4.9), (4.11), $i = 1, 2$ in order to find the strongest one. For example, it is clear that inequality (4.11) with $i = 1$ is stronger than (4.11) with $i = 2$ if $\sigma_1 \leq \sigma_2$. However, we avoid such analyses and use the bounds in the form described above.

(ii) *Upper bounds in terms of the Y-transformation of the effective moduli*

We now prove similar upper bounds on the Y-transformation of the effective moduli for a composite of two badly ordered phases. The procedure is almost identical to the discussion above and therefore we omit superfluous details.

Let consider the functional

$$I_{\tau J} = \alpha_0 \cdot \mathbf{D}_*^{\tau J} \cdot \alpha_0 \quad (4.15)$$

associated with a matrix

$$\begin{aligned} \mathbf{D}_*^{\tau J} &= \begin{pmatrix} \mathbf{A}\left(\frac{1}{3\kappa_*}, \frac{1}{2\mu_*}, \infty\right) & 0 \\ 0 & \mathbf{A}(1/\sigma_*, 1/\sigma_*, 1/\sigma_*) \end{pmatrix} \\ &= \begin{pmatrix} 1/3\kappa_* & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/2\mu_* & 0 & 0 & 0 & 0 \\ 0 & 0 & \infty & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/\sigma_* & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/\sigma_* & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/\sigma_* \end{pmatrix} \end{aligned} \quad (4.16)$$

and the vector

$$\alpha_0 = \begin{pmatrix} \tau_h & \tau_s & 0 & \mathbf{J}_h & \mathbf{J}_s & \mathbf{J}_a \end{pmatrix} \quad (4.17)$$

Remark 9. Such a representation looks ambiguous, because it includes the multiplication of the antisymmetric part of the stress tensor (that is a zero tensor) and infinity in the corresponding place of the compliance matrix. We can simply ignore the third line and column of the matrix $\mathbf{D}_*^{\tau J}$ and the third element of the vector α , but we choose such a representation to make it similar to what was done for the functional $I_{\zeta E}$.

It follows from (3.15) that the matrix

$$\mathbf{T}^{\tau J} = \begin{pmatrix} \mathbf{A}(-t_1, 2t_1, 0) & \mathbf{A}(-t_3, 2t_3, 0) \\ \mathbf{A}(-t_3, 2t_3, 0) & \mathbf{A}(-t_2, 2t_2, 0) \end{pmatrix} = \begin{pmatrix} -t_1 & 0 & 0 & -t_3 & 0 & 0 \\ 0 & 2t_1 & 0 & 0 & 2t_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -t_3 & 0 & 0 & -t_2 & 0 & 0 \\ 0 & 2t_3 & 0 & 0 & 2t_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (4.18)$$

is associated with the *quasi-convex* quadratic form $\phi_{\tau J}(\tau, \mathbf{J}, t_1, t_2, t_3)$ of the pair of

tensors $\boldsymbol{\tau}$ and \boldsymbol{J} if

$$t_1 \geq 0, \quad t_2 \geq 0, \quad (4.19)$$

and

$$t_1 t_2 - t_3^2 \geq 0. \quad (4.20)$$

Indeed, this form is equal to the following sum of functions:

$$\phi_{\tau J}(\boldsymbol{\tau}, \boldsymbol{J}, t_1, t_2, t_3) = \phi_{JJ}(\boldsymbol{\tau}, \boldsymbol{\tau}, t'_1) + \phi_{JJ}(\boldsymbol{J}, \boldsymbol{J}, t'_2) + \phi_{JJ}(a\boldsymbol{\tau} + b\boldsymbol{J}, a\boldsymbol{\tau} + b\boldsymbol{J}, t'_3), \quad (4.21)$$

where quadratic form ϕ_{JJ} is defined by (3.15), a and b are arbitrary constants, and

$$t_1 = t'_1 + a^2 t'_3, \quad t_2 = t'_2 + b^2 t'_3, \quad t_3 = ab t'_3. \quad (4.22)$$

Each term in the sum is quasi-convex provided the conditions $t'_i \geq 0$, $i = 1, 2, 3$. This proves the quasi-convexity of the form (4.21) and leads to the conditions (4.19) and (4.20). The other restrictions for the parameters t_1 , t_2 and t_3 come from the inequality

$$\boldsymbol{D}_i^{\tau J} - \boldsymbol{T}^{\tau J} \geq 0, \quad i = 1, 2. \quad (4.23)$$

The last matrix has a block-diagonal form

$$\boldsymbol{D}_i^{\tau J} - \boldsymbol{T}^{\tau J} = \boldsymbol{D}_i^{1,4} \oplus \boldsymbol{D}_i^{2,5} \oplus \boldsymbol{D}_i^{3,6}. \quad (4.24)$$

It is obvious that the matrices $\boldsymbol{D}_i^{3,6}$, $i = 1, 2$ are positive. Therefore, conditions

$$\det \boldsymbol{D}_i^{1,4} = \left(\frac{1}{3\kappa_i} + t_1 \right) \left(\frac{1}{\sigma_i} + t_2 \right) - t_3^2 \geq 0, \quad i = 1, 2, \quad (4.25)$$

$$\det \boldsymbol{D}_i^{2,5} = \left(\frac{1}{2\mu_i} - 2t_1 \right) \left(\frac{1}{\sigma_i} - 2t_2 \right) - 4t_3^2 \geq 0, \quad i = 1, 2 \quad (4.26)$$

are equivalent to (4.23). The bounds come from the inequality

$$\det[\boldsymbol{Y}(\boldsymbol{D}^{\tau J}) + \boldsymbol{T}^{\tau J}]^{1,4} = \left(\frac{1}{3y(\kappa_*)} - t_1 \right) \left(\frac{1}{y(\sigma_*)} - t_2 \right) - t_3^2 \geq 0. \quad (4.27)$$

Let Ω_T be the set of the pairs $(1/y(\sigma_*), 1/y(\kappa_*))$ that satisfy inequality (4.27) for the fixed values of the parameters t_1 , t_2 and t_3 . The bound of this set is a hyperbola in the plane $1/y(\sigma_*)$ – $1/y(\kappa_*)$, defined by the equality in (4.27) that can be written in a form (1.8) with a positive coefficient in front of the main (bilinear) term.

Conditions (4.25) are always satisfied as follows from (4.19) and (4.20), inequalities (4.26) require the pairs $(1/2\sigma_i, 3/4\mu_i)$ lie within the set Ω_T , and condition (4.20) is equivalent to saying that the pair $(0, 0)$ belongs to the set Ω_T . These are the only restrictions on the parameters, and therefore on the position of the boundary hyperbola of the set Ω_T . Analyses of these conditions for the composite with badly ordered phases leads to the following bounds:

Theorem 4.2. *The upper bound on the set of pairs $(y(\sigma_*), y(\kappa_*))$ in the plane $y(\sigma_*)$ – $y(\kappa_*)$ is given by the segment of the hyperbola*

$$\text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (\infty, \infty)],$$

which is in fact a straight line that connect the points $(2\sigma_1, \frac{4}{3}\mu_1)$ and $(2\sigma_2, \frac{4}{3}\mu_2)$.

We have proved the upper bound in terms of Y-transformations of the moduli.

Remark 10. Condition (4.2) guarantees the existence of the parameters t_1, t_2, t_3

such that the bounding hyperbola with the positive coefficient in front of the bilinear term passes through the points $(2\sigma_1, \frac{4}{3}\mu_1)$, $(2\sigma_2, \frac{4}{3}\mu_2)$, simultaneously. In this case the conditions (4.26), $i = 1, 2$, are equalities and define two equations for the three parameters t_1, t_2, t_3 . The condition (4.20) defines the third equality that allows one to define all of the coefficients.

Remark 11. To get theorem 4.2 we use the following properties of Y -transformations: $y(1/\sigma_*) = 1/y(\sigma_*)$, $y(1/\kappa_*) = 1/y(\kappa_*)$. Due to these properties, hyperbolae in the $y(1/\sigma_*)$ – $y(1/\kappa_*)$ plane correspond to hyperbolae in the $y(\sigma_*)$ – $y(\kappa_*)$ plane.

(iii) *Transformation of the conductivity–bulk modulus bounds to the σ_* – κ_* plane*

Theorems 4.1 and 4.2 for badly ordered phases can be summarized as follows.

Theorem 4.3. *In order to find bounds on the set of pairs $(y(\sigma_*), y(\kappa_*))$, one should inscribe in the $y(\sigma_*)$ – $y(\kappa_*)$ plane the four following segments of the hyperbolae:*

$$\begin{aligned} \text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_1, -\kappa_1)], \quad & \text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_2, -\kappa_2)], \\ \text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-2\sigma_1, 0)], \quad & \text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-2\sigma_2, 0)] \end{aligned}$$

and the straight line connecting the points $(2\sigma_1, \frac{4}{3}\mu_1)$ and $(2\sigma_2, \frac{4}{3}\mu_2)$. The outermost two of these curves represent the required bounds.

Remark 12. As we will see, theorem 4.3 is also valid for any composite with well-ordered phases. Therefore, it gives the bounds for the pair $(y(\sigma_*), y(\kappa_*))$ of the Y -transformations of the effective moduli. Note that in such a form the bounds do not depend explicitly on the volume fractions. They do depend on the phase volume fractions implicitly through the definition of the Y -transformations $y(\sigma_*)$ and $y(\kappa_*)$.

Now we need to transform the bounds into the plane of the actual moduli, not their Y -transformations. First we mention that Y -transformation is a fractional-linear one. Therefore, hyperbolae in the $y(\sigma_*)$ – $y(\kappa_*)$ plane correspond to the hyperbolae in the σ_* – κ_* plane. Any hyperbola can be defined by three points that it passes through. Hence, in order to transform the results into the plane of actual moduli, we need to study the correspondence between the characteristic points on the boundary hyperbolae. The straight line connecting the points $(2\sigma_1, \frac{4}{3}\mu_1)$ and $(2\sigma_2, \frac{4}{3}\mu_2)$ can be treated as the segment of the hyperbola $\text{Hyp}((2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (\infty, \infty))$ that passes through the point (∞, ∞) in the $y(\sigma_*)$ – $y(\kappa_*)$ plane. We note that

$$y(\sigma_{i*}) = 2\sigma_i, \quad y(\sigma_{i\#}) = -2\sigma_i, \quad y(\sigma_i) = -\sigma_i, \quad i = 1, 2, \quad y(\sigma_a) = \infty, \quad (4.28)$$

$$y(\kappa_{i*}) = \frac{4}{3}\mu_i, \quad y(\kappa_i) = -\kappa_i, \quad i = 1, 2, \quad y(\kappa_h) = 0, \quad y(\kappa_a) = \infty, \quad (4.29)$$

where the values σ_{i*} , $\sigma_{i\#}$, κ_{i*} $i = 1, 2$, σ_a , κ_a and κ_h are defined by equations (1.3)–(1.7). Therefore, theorem 4.3 is equivalent to theorem 1.1. It is proved here in the specific case (4.2) of badly ordered materials.

(b) *Bulk modulus–conductivity bounds for a composite of two well-ordered materials*

The proof of theorem 1.1 for the composite of two well-ordered materials is almost identical to the badly ordered case. The difference is that we need to study the functionals (3.2) and (3.3) instead of the functionals (3.1) and (3.4) and use appropriate quasi-convex quadratic forms. We leave the proof to the reader.

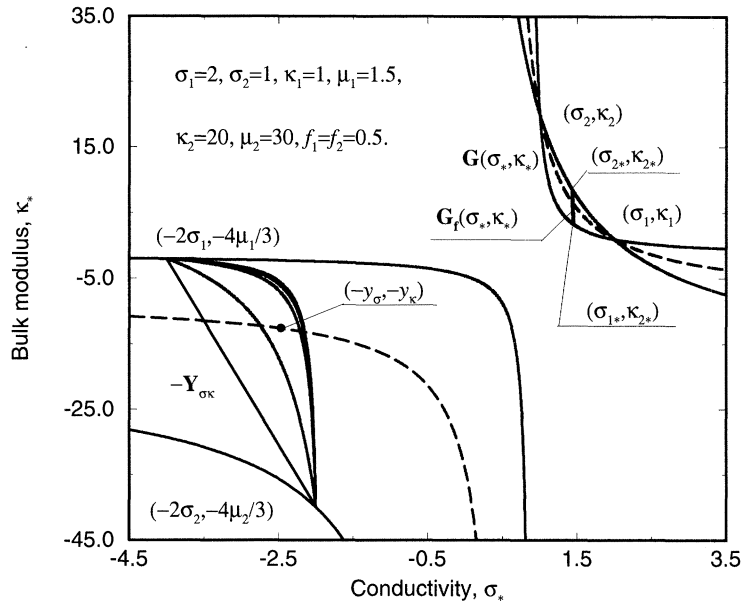


Figure 4. Construction of the conductivity–bulk modulus bounds for the composite with arbitrary phase volume fraction.

5. Cross-property bounds for arbitrary volume fractions

Theorem 1.1 deals with cross-property bounds when the volume fractions of the phases in the composite are known. Here we briefly show how to obtain analogous results when the volume fraction is unknown.

Let $G_f(\sigma_*, \kappa_*)$ represent the set of all pairs (σ_*, κ_*) that satisfy the bounds of theorem 1.1. Let $G(\sigma_*, \kappa_*)$ denote the set which is the union over volume fractions $f_1 \in [0, 1]$ of the sets $G_f(\sigma_*, \kappa_*)$, i.e.

$$G(\sigma_*, \kappa_*) = \cup_{f_1 \in [0, 1]} G_f(\sigma_*, \kappa_*). \quad (5.1)$$

It is obvious that this set contains the pair of values of the effective properties of any composite structure. In order to find this set, we use an approach that is similar to one used by Gibiansky & Lakes (1993). The procedure is illustrated in figure 4, where the sets $G_f(\sigma_*, \kappa_*)$ and $G(\sigma_*, \kappa_*)$ are shown for the following values of the parameters:

$$\sigma_1 = 1, \quad \sigma_2 = 1, \quad \kappa_1 = \mu_1 = 1, \quad \kappa_2 = \mu_2 = 20, \quad f_1 = f_2 = 0.5. \quad (5.2)$$

Note that the set $G_f(\sigma_*, \kappa_*)$ degenerates into one bold line on the scale of figure 4.

First, we recall that the effective moduli of a composite can be expressed in terms of their Y -transformations as follows:

$$\sigma_* = f_1 \sigma_1 + f_2 \sigma_2 - \frac{f_1 f_2 (\sigma_1 - \sigma_2)^2}{f_2 \sigma_1 + f_1 \sigma_2 + y_\sigma} = F_\sigma(y_\sigma), \quad (5.3)$$

$$\kappa_* = f_1 \kappa_1 + f_2 \kappa_2 - \frac{f_1 f_2 (\kappa_1 - \kappa_2)^2}{f_1 \kappa_2 + f_2 \kappa_1 + y_\kappa} = F_\kappa(y_\kappa). \quad (5.4)$$

Here y_σ and y_κ are the Y -transformations of the effective conductivity and the bulk modulus, respectively. Let us fix some values $y_\sigma = y(\sigma_*)$ and $y_\kappa = y(\kappa_*)$ and consider the trajectories in the $\sigma_*-\kappa_*$ plane of the point (σ_*, κ_*) as the volume fraction f_1 is varied in the interval $f_1 \in [0, 1]$. One can check that equations (5.3), (5.4) ($f_1 \in [0, 1]$) represent a segment of a hyperbola in the $\sigma_*-\kappa_*$ plane. This hyperbola (dashed line of figure 4) passes through the points (σ_1, κ_1) (when $f_1 = 1$), (σ_2, κ_2) (when $f_1 = 0$) and $(-y_\sigma, -y_\kappa)$ (when $f_1 = \infty$). The position of the point $(-y_\sigma, -y_\kappa)$ is restricted by our cross-property bounds (theorem 4.3). Namely, the point $(-y_\sigma, -y_\kappa)$ should lie within the set $-Y_{\sigma\kappa}$ (see figure 4) that is restricted by the outermost pair of the five curves, that are four segments of the hyperbolae

$$\begin{aligned} &\text{Hyp}[(-2\sigma_1, -\frac{4}{3}\mu_1), (-2\sigma_2, -\frac{4}{3}\kappa_2), (\sigma_1, \kappa_1)], \\ &\text{Hyp}[(-2\sigma_1, -\frac{4}{3}\mu_1), (-2\sigma_2, -\frac{4}{3}\mu_2), (\sigma_2, \kappa_2)], \\ &\text{Hyp}[(-2\sigma_1, -\frac{4}{3}\mu_1), (-2\sigma_2, -\frac{4}{3}\mu_2), (2\sigma_1, 0)], \\ &\text{Hyp}[(-2\sigma_1, -\frac{4}{3}\mu_1), (-2\sigma_2, -\frac{4}{3}\mu_2), (2\sigma_2, 0)], \end{aligned}$$

and the straight line connecting the points $(-2\sigma_1, -\frac{4}{3}\mu_1)$ and $(-2\sigma_2, -\frac{4}{3}\mu_2)$.

It is clear that in order to find bounds on the effective properties of a composite for arbitrary volume fractions, we need to take the union of all segments of the hyperbolae that pass through the points of the original materials (σ_1, κ_1) and (σ_2, κ_2) and when extended cross the set $-Y_{\sigma\kappa}$. One can see that the bounds of this union are given by two extremal hyperbolae that pass through the points of the original materials and only touch the set $-Y_{\sigma\kappa}$ (see figure 4). It remains to find the exact expressions for these extremal hyperbolae. We will not go into the details of these long but straightforward calculations.

6. Optimal microstructures

In this section we describe briefly the microstructures that are known to correspond to the points on the boundary of the set $G_f(\sigma_*, \kappa_*)$. Because any of the hyperbolae segments mentioned in theorem 1.1 may form the boundary, we are interested in finding the composite that corresponds to the points on any of these segments. First note that the corner points of the set $G_f(\sigma_*, \kappa_*)$ correspond to the assemblages of coated spheres introduced by Hashin & Shtrikman (1962, 1963). Namely, the point $A = (\sigma_{1*}, \kappa_{1*})$ (see figure 1) corresponds to the structure that has a core of phase 2 surrounded by a coating of phase 1, whereas the point $B = (\sigma_{2*}, \kappa_{2*})$ corresponds to the composite that has a core of phase 1 surrounded by a coating of phase 2.

Let us next investigate assemblages of doubly coated spheres (Schulgasser 1977): these are natural candidates since such assemblages were found to exhibit extremal properties for the complex conductivity bounds (Milton 1981) and complex viscoelasticity bounds (Gibiansky & Milton 1993). To prepare such an assemblage, we first construct a prototype coated sphere from the initial materials with phase 1 in the core and phase 2 in the coating. In the second step, we surround the prototype coated sphere with an additional coating of phase 1. One can check (similar to Milton (1981) and Gibiansky & Milton (1993)) that the conductivity–bulk modulus pair (σ_*, κ_*) of an assemblage of these doubly coated spheres lie on the curve $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_1, \kappa_1)]$. By interchanging the roles of phase 1 and 2 it is clear that points on the curve $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_2, \kappa_2)]$ correspond to the conductivity and bulk modulus of doubly coated spheres with a core of phase 2

surrounded by successive coatings of phase 1 and 2. Therefore, if the bounds on the pair (σ_*, κ_*) are described either by $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_1, \kappa_1)]$ or by $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_2, \kappa_2)]$, then these bounds are optimal.

More complicated structures are needed to attain points on the other hyperbolae. We recall here the results by Milton (1981) for the three-dimensional complex conductivity problem and the results by Gibiansky & Milton (1993) for the three-dimensional viscoelasticity problem. There the bounds were given by the outermost of circular arcs. Two of these arcs correspond to the doubly coated sphere geometries, while five points on the other arc were found to correspond to particular geometries. In the problem under study, the situation is very similar except circles in the complex plane are replaced by hyperbolae in the conductivity–bulk modulus plane. The same five microstructures that were optimal in the aforementioned papers are optimal for our problem as well, i.e. they lie on the line $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_a, \kappa_a)]$. Two of the points correspond to the coated sphere geometries and the remaining three points are obtained by a two-step process. In the first step, an anisotropic composite is built either by layering the two phases together or by constructing a coated cylinder assemblage with either phase 1 or 2 as core (Hashin 1965). In the second step, a construction of Schulgasser (1976*b*) is used to build an isotropic polycrystalline material from the composite prepared in the first step, which is effectively treated as a pure crystal. (This two-step procedure starting from a simple laminate was also used by Schulgasser (1976*a*); for further details see Gibiansky & Milton (1993).)

We may summarize our findings as follows: for any fixed volume fraction f_1 there exist structures that correspond to any point on the segments of the hyperbolae $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_1, \kappa_1)]$ and $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_2, \kappa_2)]$, and to five points on the curve $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_a, \kappa_a)]$. At the moment we do not know structures that correspond to any point on the curves $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_{1\#}, \kappa_h)]$ and $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}), (\sigma_{2*}, \kappa_{2*}), (\sigma_{2\#}, \kappa_h)]$ (except end points $A = (\sigma_{1*}, \kappa_{1*})$ and $B = (\sigma_{2*}, \kappa_{2*})$).

7. Applications and discussion

In this section we apply our cross-property bounds given in §1 (theorem 1.1) to some special limiting cases of the phase properties. We also examine our bounds for specific microgeometries, including regular and random arrays of spheres and hierarchical geometries corresponding to effective-medium theories. We begin with a comparison of our bounds to the bounds of Berryman & Milton (1988).

(a) Comparison of our results with Berryman–Milton bounds

Berryman & Milton (1988) applied an entirely different method to obtain the cross-property bounds on the pairs (σ_*, κ_*) . In order to find such bounds they used three-point bounds on the effective conductivity and elastic moduli that depend on certain microgeometrical parameters of the composite. Excluding these parameters from the conductivity and elastic moduli bounds, they were able to obtain bounds on the effective bulk and shear moduli of the composite in terms of the effective conductivity. We, however, restrict ourselves to the (σ_*, κ_*) bounds only.

It is helpful to formulate the Berryman–Milton bounds in a form similar to our theorem 1.1. First note that three-point bounds on the conductivity and bulk modulus of isotropic composites (see, for example, Beran 1968; Milton 1984) can be written

as

$$2\zeta_1\sigma_1 + 2\zeta_2\sigma_2 - \frac{4\zeta_1\zeta_2(\sigma_1 - \sigma_2)^2}{2\zeta_2\sigma_1 + 2\zeta_1\sigma_2 + \sigma_{\min}} \leq y(\sigma_*) \leq 2(\zeta_1\sigma_1 + \zeta_2\sigma_2), \quad (7.1)$$

$$\left(\frac{3\zeta_1}{4\mu_1} + \frac{3\zeta_2}{4\mu_2} \right)^{-1} \leq y(\kappa_*) \leq \frac{4}{3}(\zeta_1\mu_1 + \zeta_2\mu_2). \quad (7.2)$$

Here ζ_1 and $\zeta_2 = 1 - \zeta_1$ are certain integrals over three-point correlation functions. The quantities $y(\sigma_*)$ and $y(\kappa_*)$ are the Y -transformations of the conductivity and bulk modulus, respectively, and $\sigma_{\min} = \min\{\sigma_1, \sigma_2\}$ is the minimal phase conductivity. The key idea of Berryman & Milton (1988) was to exclude ζ_1 from these relations in order to get bounds on the effective bulk modulus in terms of the effective conductivity.

For a fixed value ζ_1 , the pair $(y(\sigma_*), y(\kappa_*))$ should lie within the square (7.1), (7.2) in the $y(\sigma_*)$ – $y(\kappa_*)$ plane. When the value ζ_1 changes within the interval $[0, 1]$, this square traces out the set that obviously contains the pair $(y(\sigma_*), y(\kappa_*))$ of any composite. The bounds of this set are traced out by certain of the corner points of the square (7.1), (7.2). They are given by the outermost of the four curves that are three segments of the hyperbolae

$$\begin{aligned} &\text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_{\min}, 0)], \quad \text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_{\min}, \infty)], \\ &\text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (\infty, 0)], \end{aligned}$$

and the straight line connecting the points $(2\sigma_1, \frac{4}{3}\mu_1)$ and $(2\sigma_2, \frac{4}{3}\mu_2)$. Note that σ_{\min} can take the value σ_1 or σ_2 , depending on which of them is smaller. Now we can formulate the Berryman–Milton bounds in the following form.

Theorem 7.1. (Berryman–Milton bounds). *In order to find bounds on the set of pairs $(y(\sigma_*), y(\kappa_*))$, one should inscribe in the $y(\sigma_*)$ – $y(\kappa_*)$ plane the following five segments of the hyperbolae:*

$$\begin{aligned} &\text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_1, 0)], \quad \text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_2, 0)], \\ &\text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_1, \infty)], \quad \text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_2, \infty)], \\ &\text{Hyp}[(2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (\infty, 0)], \end{aligned}$$

and the straight line connecting the points $(2\sigma_1, \frac{4}{3}\mu_1)$ and $(2\sigma_2, \frac{4}{3}\mu_2)$. The outermost two of these curves represent the Berryman–Milton bounds.

Let us compare our bounds (in the form of theorem 4.3 for the Y -transformation of the effective moduli) with the Berryman–Milton bounds in the form of theorem 7.1. The straight line connecting the points $(2\sigma_1, \frac{4}{3}\mu_1)$ and $(2\sigma_2, \frac{4}{3}\mu_2)$ is present in both theorems. If this line forms one of the bounds, then this bound is the same for both theorems 4.3 and 7.1. One can check that each of the other curves that are described in theorem 4.3 lie between some of the curves defined by theorem 7.1. Indeed, the curve

$$\text{Hyp}((2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_1, -\kappa_1))$$

lies between the curves

$$\text{Hyp}((2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_1, 0)) \quad \text{and} \quad \text{Hyp}((2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_1, \infty)).$$

The curve

$$\text{Hyp}((2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_2, -\kappa_2))$$

lies between the curves

$$\text{Hyp}((2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_2, 0)) \quad \text{and} \quad \text{Hyp}((2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_2, \infty)).$$

The curve

$$\text{Hyp}((2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-2\sigma_1, 0))$$

lies between the curves

$$\text{Hyp}((2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_1, 0)) \quad \text{and} \quad \text{Hyp}((2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (\infty, 0)).$$

The curve

$$\text{Hyp}((2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-2\sigma_2, 0))$$

lies between the curves

$$\text{Hyp}((2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (-\sigma_2, 0)) \quad \text{and} \quad \text{Hyp}((2\sigma_1, \frac{4}{3}\mu_1), (2\sigma_2, \frac{4}{3}\mu_2), (\infty, 0)).$$

Therefore, in general, our bounds are tighter than those of Berryman & Milton (1988). Figures 1 and 2 illustrate this difference.

(b) Equal phase moduli

Consider our bounds for some particular values of the parameters of the phases. Let us begin with composites possessing *equal shear moduli* $\mu_1 = \mu_2 = \mu$. This is a trivial instance because both effective elastic moduli do not depend on the microstructure (see, for example, Christensen 1979) and therefore are not connected with the effective conductivity.

(c) Superrigid superconducting phase

Let assume that *one of the phases is super-rigid and superconducting*, i.e. $\kappa_2/\kappa_1 = \infty$, $\mu_2/\mu_1 = \infty$ and $\sigma_2/\sigma_1 = \infty$. The boundary hyperbolae in this extreme case degenerate into straight lines and the bounds for fixed $f_1 = 1 - f_2$ simply as

$$\sigma_* \geq \sigma_{1*}^\infty, \quad \kappa_{1*}^\infty \leq \kappa_* \leq \kappa_{1*}^\infty + \max \left[\frac{3\kappa_1 + 4\mu_1}{9\sigma_1}, \frac{6\kappa_2\mu_2}{(3\kappa_2 + 4\mu_2)\sigma_2}, \frac{2\mu_2}{3\sigma_2} \right] (\sigma_* - \sigma_{1*}^\infty), \quad (7.3)$$

where

$$\sigma_{1*}^\infty = \frac{1 + 2f_2}{f_1} \sigma_1, \quad \kappa_{1*}^\infty = \frac{3\kappa_1 + 4f_2\mu_1}{3f_1}. \quad (7.4)$$

Note that the lower bound on the elastic moduli is independent of the conductivity and coincides with the corresponding Hashin–Shtrikman lower bound. For arbitrary volume fractions $f_1 = 1 - f_2$, relations (7.3), (7.4) reveal that the following inequalities hold:

$$\sigma_* \geq \sigma_1, \quad \kappa_1 \leq \kappa_* \leq \kappa_1 + \max \left[\frac{3\kappa_1 + 4\mu_1}{9\sigma_1}, \frac{6\kappa_2\mu_2}{(3\kappa_2 + 4\mu_2)\sigma_2}, \frac{2\mu_2}{3\sigma_2} \right] (\sigma_* - \sigma_1). \quad (7.5)$$

At first glance it appears odd that the bounds can depend on the ratio of the infinite moduli of the ideal phase. This occurs because the addition to the composite of an infinitesimal amount (of order $1/\kappa_2$ or $1/\sigma_2$) of a super-rigid superconducting phase-2 material can lead to changes in the possible range of the effective properties, as we now describe. The upper bounds defined by each of the equations (7.3), (7.5)

represent straight lines whose slopes depend on the ratios of the quantities under the maximum operation. The line (7.3) with the slope $\tan(\alpha_1) = (4\kappa_1 + 3\mu_1)/9\sigma_1$ is realizable by the assemblages of doubly coated spheres where the core and the external coating are made of the first material and the ideal phase is placed in the intermediate coating. The line (7.5) with the same slope corresponds to the Hashin–Shtrikman coated-spheres assemblages. The lines (7.3) and (7.5) with the slope $\tan(\alpha_2) = 6\kappa_2\mu_2/(3\kappa_2 + 4\mu_2)\sigma_2$ correspond to the assemblages of doubly or singly coated spheres with an inverse order of the materials when the thickness of the external coating is extremely small (i.e. for the effective conductivity and bulk modulus to be finite it should be of the order of $1/\mu_2$ and $1/\sigma_2$). Note that $\tan(\alpha_2) \geq \tan(\alpha_3) = 2\mu_2/3\sigma_2$ if $\nu_2 \geq 0$.

Remark 13. Unlike Hashin–Shtrikman and Berryman–Milton upper bounds on κ_* , the upper bounds in (7.3), (7.5) do not diverge to infinity if σ_* remains finite in this infinite-contrast case. The lower bound in (7.3) is trivial and coincides with the lower Hashin–Shtrikman bound for κ_* .

(d) *Void or fluid phase*

(i) *Perfectly insulating void phase*

Let us now assume that *one of the phases is composed of voids*, i.e. $\kappa_2/\kappa_1 = 0$, $\mu_2/\mu_1 = 0$, $\sigma_2/\sigma_1 = 0$. It is convenient to present the results in the inverse coordinates, i.e. in the $1/\sigma_*$ – $1/\kappa_*$ plane. For a fixed volume fraction, the bounds are given simply as

$$1/\sigma_* \geq 1/\sigma_{1*}^0, \quad 1/\kappa_* \geq 1/\kappa_{1*}^0 + \min \left[\frac{(3\kappa_1 + 4\mu_1)\sigma_1}{6\kappa_1\mu_1}, \frac{9\sigma_2}{3\kappa_2 + 4\mu_2}, \frac{3\sigma_1}{2\mu_1} \right] (1/\sigma_* - 1/\sigma_{1*}^0), \quad (7.6)$$

where

$$1/\sigma_{1*}^0 = \frac{1 + f_2}{2f_1\sigma_1}, \quad 1/\kappa_{1*}^0 = \frac{4\mu_1 + 3f_2\kappa_1}{4f_1\kappa_1\mu_1}. \quad (7.7)$$

For arbitrary volume fractions, the bounds are given by

$$1/\sigma_* \geq 1/\sigma_1, \quad 1/\kappa_* \geq 1/\kappa_1 + \min \left[\frac{(3\kappa_1 + 4\mu_1)\sigma_1}{6\kappa_1\mu_1}, \frac{9\sigma_2}{3\kappa_2 + 4\mu_2}, \frac{3\sigma_1}{2\mu_1} \right] (1/\sigma_* - 1/\sigma_1), \quad (7.8)$$

The lower bound in (7.6) is trivial and equal to zero; it coincides with the lower Hashin–Shtrikman bound for κ_* . Our upper bounds provide improvement upon the Hashin–Shtrikman and Berryman–Milton upper bounds (which are equal to one another for such a choice of the parameters).

The upper bounds defined by each of the equations (7.6), (7.8) represent straight lines in the $1/\sigma_*$ – $1/\kappa_*$ plane whose slopes depend on the ratios of the quantities under the minimum operation. The line (7.6) with the slope $\tan(\alpha'_1) = (3\kappa_1 + 4\mu_1)\sigma_1/6\kappa_1\mu_1$ is realizable by the assemblages of doubly coated spheres, where the core and the external coating are made of the first material and the ideal phase is placed in the intermediate coating. The line (7.8) with the same slope corresponds to the Hashin–Shtrikman coated spheres assemblages. The lines (7.6) and (7.8) with the slopes $\tan(\alpha'_2) = 9\sigma_2/(3\kappa_2 + 4\mu_2)$ correspond to the assemblages of doubly or singly coated spheres with inverse order of the materials when the thickness of external coating is extremely small (i.e. for the effective conductivity and the bulk modulus to be finite it should be of the order of μ_2 and σ_2). Note that $\tan(\alpha'_1) \leq \tan(\alpha'_3) = 3\sigma_1/2\mu_1$ if $\nu_1 \geq 0$.

(ii) *Conducting gas phase*

Let us now consider the case when one phase is a gas phase such that it possesses zero elastic moduli but finite conductivity, i.e.

$$\kappa_2/\kappa_1 = 0, \quad \mu_2/\mu_1 = 0, \quad \text{but } \sigma_2/\sigma_1 \neq 0. \quad (7.9)$$

It is easy to verify that the lower bound is trivial and equal to zero but the upper bound is non-trivial. The pair (σ_*, κ_*) for any such composite must lie within the set bounded by the outermost of the curves

$$\begin{aligned} \kappa_* = 0, \quad \sigma_* \in [\sigma_{1*}, \sigma_{2*}], \quad \sigma_* = \sigma_{1*}, \quad \kappa_* \in [0, \kappa_{1*}^0], \\ \text{Hyp}[(\sigma_{1*}, \kappa_{1*}^0), (\sigma_{2*}, 0), (\sigma_1, \kappa_1)], \quad \text{Hyp}[(\sigma_{1*}, \kappa_{1*}^0), (\sigma_{2*}, 0), (\sigma_a, \kappa_a)]. \end{aligned}$$

For this case, σ_{1*} and σ_{2*} are given by relations (1.3), κ_{1*}^0 is defined by (7.7), and $\kappa_{2*} = 0$.

The lower bound is optimal. Specifically, assemblages of doubly coated spheres with an inner core and outer concentric shell made up of phase-2 material correspond to the points on the line $\kappa_* = 0$ when the thickness of the outer shell is finite, or to the line $\sigma_* = \sigma_{1*}$ when the thickness of the outer shell is infinitely small (of the order of κ_2 and μ_2). Assemblages of doubly coated spheres with an inner core and outer concentric shell made of the material with finite properties correspond to the upper bulk modulus bound if it is given by the curve $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}^0), (\sigma_{2*}, 0), (\sigma_1, \kappa_1)]$. The other curve $\text{Hyp}[(\sigma_{1*}, \kappa_{1*}^0), (\sigma_{2*}, 0), (\sigma_a, \kappa_a)]$ has five attainable points (see § 6).

 (iii) *Conducting liquid in an insulating solid*

Consider now the instance when phase 2 is a conducting liquid that fills the pores in some insulating solid material such that

$$\sigma_1/\sigma_2 = 0, \quad \mu_1/\mu_2 = \infty, \quad (7.10)$$

or

$$\sigma_1 = 0, \quad \mu_2 = 0, \quad (7.11)$$

and the rest of the moduli have finite values. In this case, the conductivity–bulk modulus bounds stated in theorem 1.1 are described by the curves

$$\sigma_* = 0, \quad \kappa_* \in [\kappa_h, \kappa_{1*}]; \quad \kappa_* = \kappa_h, \quad \sigma_* \in [0, \sigma_{2*}]; \quad \text{Hyp}[(0, \kappa_{1*}), (\sigma_{2*}, \kappa_h), (\sigma_a, \kappa_a)].$$

Here σ_{2*} and σ_a are given by equations (1.3), (1.6) and are equal to

$$\sigma_{2*} = \frac{2f_2\sigma_2}{2+f_1}, \quad \sigma_a = f_2\sigma_2. \quad (7.12)$$

The quantities κ_{1*} and κ_a are given by equations (1.5) and (1.7), respectively. Note that $\sigma_{1*} = 0$ and $\kappa_{2*} = \kappa_h$ for the choice (7.11) of materials.

Assemblages of doubly coated spheres with an inner core and outer concentric shell made up of phase-1 material correspond to the points on the line $\sigma_* = 0$ when the thickness of the outer shell is finite, or to the line $\kappa_* = \kappa_h$ when the thickness of the outer shell is infinitely small (of the order of σ_1). There exist composites that correspond to five of the boundary points of the curve $\text{Hyp}[(0, \kappa_{1*}), (\sigma_{2*}, \kappa_h), (\sigma_a, \kappa_a)]$ (see § 6).

(e) *Bounds for arrays of spheres*(i) *Cubic arrays of spheres*

How sharp are our cross-property estimates given an exact determination of one of the effective properties? To examine this question we first employ the exact results of McKenzie *et al.* (1978) for the effective conductivity of cubic arrays of spheres and our cross-property relations in order to obtain bounds on the effective bulk modulus. (The bounds of theorem 1.1 are applicable to the bulk modulus of such a composite, although it is not isotropic but cubic symmetric.) We then compare our bounds on κ_* with the results of Nunan & Keller (1984) for the elastic moduli of such a cubic symmetric composite with an effective stiffness tensor \mathbf{C} , expressible as

$$C_{ijkl} = (\lambda_1 + \mu_1\gamma)\delta_{ij}\delta_{kl} + \mu_1(1 + \beta)(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + 2\mu_1(\alpha - \beta)\delta_{ijkl}. \quad (7.13)$$

Here $\lambda_1 = \kappa_1 - \frac{2}{3}\mu_1$ is the Lamé constant; δ_{ijkl} is equal to one if all the subscripts are equal and zero otherwise; and α , β and γ are functions of the inclusion volume fraction tabulated by Nunan & Keller (1984). As follows from (7.13), the effective bulk modulus of such a composite (in terms of the functions α and γ) is given by

$$\kappa_* = \kappa_1 + \mu_1(\gamma + \frac{2}{3}\alpha). \quad (7.14)$$

In particular, we study face-centred cubic arrays of superconducting super-rigid inclusions (phase 2) in a matrix in which $\kappa_2/\kappa_1 = \infty$, $\mu_2/\mu_1 = \infty$ and $\nu_1 = 0.3$ or $\nu_1 = 0.45$. The bounds in this instance are given by the relations (7.3). We make the additional but weak assumption that phase 1 determines the slope of the upper bound in (7.3), i.e.

$$\frac{3\kappa_1 + 4\mu_1}{9\sigma_1} \geq \frac{6\kappa_2\mu_2}{(3\kappa_2 + 4\mu_2)\sigma_2}, \quad \frac{3\kappa_1 + 4\mu_1}{9\sigma_1} \geq \frac{9\mu_2}{3\sigma_2}. \quad (7.15)$$

Figure 5 summarizes our findings. Note that only the upper bound contains conductivity information. We see that for volume fractions in the range $f_2 \leq 0.5$, our bounds predict the bulk modulus of the composite almost exactly. For higher volume fractions, agreement with the data of Nunan & Keller (1984) is still very good.

It is important to emphasize that conventional variational upper bounds on the effective properties (such as Hashin–Shtrikman), as well as the Berryman–Milton bound, here diverge to infinity as they are not able to incorporate the information that the super-rigid phase is in fact disconnected. In contrast, *our cross-property upper bound uses the important topological information that the infinite-contrast phase is disconnected through information on the conductivity.*

(ii) *Random distribution of spheres*

Conductivity data for ‘equilibrium’ distributions of mutually impenetrable spheres have been obtained by Kim & Torquato (1990) for several volume fractions and contrast ratios. We are not aware of elastic moduli data for the same random array. It is of interest to see how well our cross-property relations predict the elastic moduli in this instance. Let us consider the case of random superconducting spheres ($\sigma_2/\sigma_1 = \infty$) for several volume fractions and take $\kappa_2/\kappa_1 = 10$, $\mu_1/\kappa_1 = \mu_2/\kappa_2 = 0.4$. Note that unlike the previous example, κ_2/κ_1 is finite. Figure 6 shows the bulk modulus-conductivity bounds. One can see that they are quite sharp. Our cross-property *upper bound* provides substantial improvement over the Hashin–Shtrikman *upper bound* on κ_* , which of course remains finite in this instance.

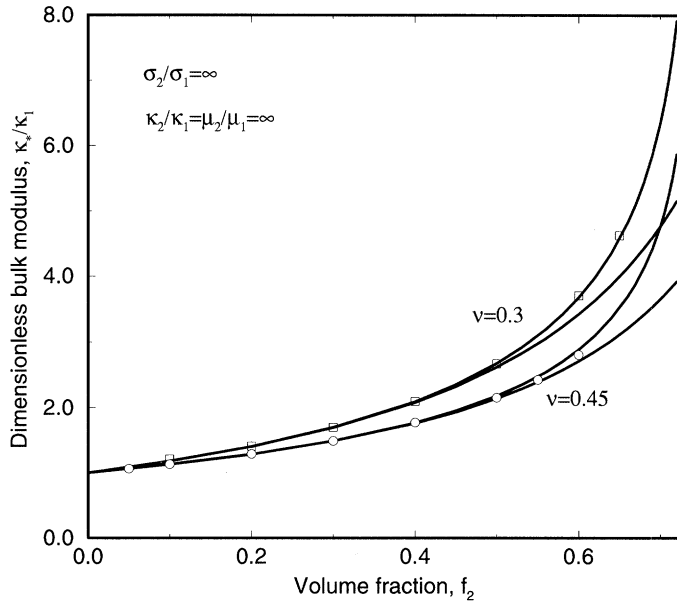


Figure 5. Comparison of the cross-property bounds on the bulk modulus (solid curves) with exact bulk modulus data by Nunan & Keller (1984) (circles and squares) for $\nu = 0.3$ and $\nu = 0.45$ for a super-rigid superconducting face-centred cubic array of spherical inclusions. The bounds of theorem 1.1 in the form of (7.3) are calculated using the exact conductivity data of McKenzie *et al.* (1978).

(iii) *Random arrays of non-touching spheres*

We will also apply our results to bounds on the effective moduli of random arrays of *non-touching* inclusions in which the phase contrast is large. Two different approaches were used to construct non-trivial bounds on the moduli of such high-contrast arrays. One method, referred to as the ‘security-spheres’ approach, uses classical variational principles to obtain bounds in terms of the *nearest-neighbour distribution function* (Keller *et al.* 1967; Rubinstein & Torquato 1988; Torquato & Rubinstein 1991). The other makes use of the analytical properties of the effective moduli (Bruno 1991; Bruno & Leo 1993). Depending on the value of the minimum interparticle distance and the physical problem, one of the two aforementioned methods can yield better bounds than the other.

We consider a composite of identical spheres of diameter d in a matrix. The arrangement is such that these inclusions are closely packed but with an additional condition that there is a minimum interparticle distance $d(1 - q)/q$ between any two sphere surfaces, where q is the separation ratio. Random arrays of closely packed spheres fill around 60% of the volume and, hence, the inclusion volume fraction is given by

$$f_2 = 0.6q^3. \quad (7.16)$$

Here we use the bounds on the effective conductivity of such a composite that were derived by Bruno (1991) and our results to find bounds on the effective bulk modulus. We then compare these bounds with the corresponding bulk modulus bounds of

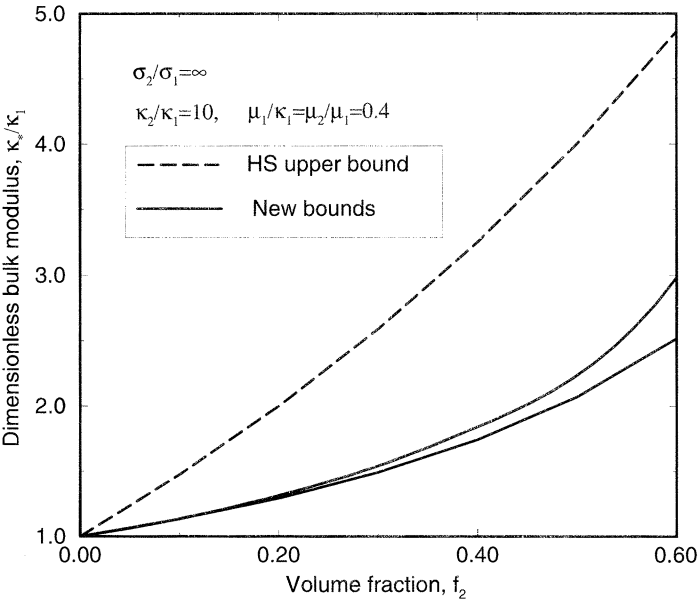


Figure 6. Cross-property bounds on the effective bulk modulus κ_* for a superconducting random array of spherical inclusions with $\kappa_2/\kappa_1 = 10$, $\mu_1/\kappa_1 = \mu_2/\kappa_2 = 0.4$, given the exact effective conductivity data given by Kim & Torquato (1990). Included is the Hashin–Shtrikman upper bound. The Hashin–Shtrikman lower bound coincides with our lower bound in this case.

Table 1. Comparison of bounds on the effective bulk modulus of random arrays of non-touching spheres with superconducting super-rigid inclusions (see 7.17)

q	f_2	V	κ_u	W	B_u
0.10	0.000 600	1.001 80	1.000 970	1.000 999	1.000 970
0.20	0.004 800	1.014 49	1.007 802	1.008 010	1.007 816
0.30	0.016 200	1.049 59	1.026 702	1.027 217	1.026 895
0.40	0.038 400	1.120 97	1.065 138	1.065 388	1.066 272
0.50	0.075 000	1.248 41	1.133 759	1.134 720	1.138 462
0.60	0.129 600	1.465 25	1.250 519	1.265 242	1.267 033
0.70	0.205 800	1.852 62	1.459 103	1.539 267	1.506 006
0.80	0.307 200	2.663 24	1.895 591	2.202 338	2.016 898
0.90	0.437 400	5.143 29	3.231 002	4.416 647	3.607 267
0.93	0.482 614	7.280 52	4.381 818	6.380 136	4.984 848
0.96	0.530 842	12.6322	7.263 492	11.319 122	8.439 560
0.99	0.582 179	50.1269	27.452 946	45.833 070	32.663 703

Bruno & Leo (1993) for this composite. We use the results of Bruno (1991) and Bruno & Leo (1993), since they provide the most comprehensive data for both the conductivity and bulk modulus.

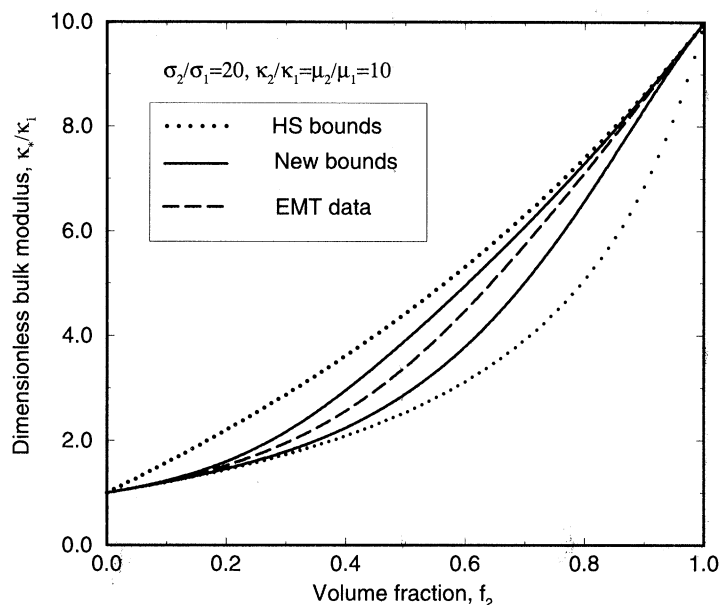


Figure 7. Comparison of the cross-property bounds on the bulk modulus (solid curves) with the exact result (7.19)–(7.20) (dashed lines) for the bulk modulus of the effective-medium geometry. Bounds of theorem 1.1 are calculated using the exact conductivity result (7.18). Dotted lines are the Hashin–Shtrikman bounds.

Table 1 summarizes our findings for the case of superconducting super-rigid inclusions ($\sigma_2/\sigma_1 = \infty$, $\kappa_2/\kappa_1 = \mu_2/\mu_1 = \infty$) in a matrix with moduli given by

$$\sigma_1 = 1, \quad \kappa_1 = 1, \quad \nu_1 = 0.3. \quad (7.17)$$

The first and second columns of table 1 give the separation ratio q and the inclusion volume fraction $f_2 = 0.6q^3$, respectively. The next column gives the upper bound V for the effective conductivity, as given in table 2b of Bruno (1991). The fourth column shows the upper bound κ_u that follow from relations (7.3) by using the conductivity value V . The last two columns show the best previously known upper bounds on the bulk modulus, as given in table 8 of Bruno & Leo (1993). The bound W was obtained using the analytical method and the bound B_u was derived using the security-spheres approach. As we see, our cross-property relations allow us to improve upon these known bounds. Note that *lower bounds* of Bruno & Leo (1993) on the effective bulk modulus and our lower bound that follows from (7.3) coincide and are equal here to the Hashin–Shtrikman lower bound.

(f) *Effective-medium theory geometries*

It is useful to examine our cross-property bounds for structures in which the effective properties are known exactly analytically. One such example is the class of structures that correspond to the effective-medium theories (see Bruggeman 1935; Budiansky 1965), in which the effective properties are given by the solutions of the equations

$$f_1 \frac{\sigma_1 - \sigma_e}{\sigma_1 + 2\sigma_e} + f_2 \frac{\sigma_2 - \sigma_e}{\sigma_2 + 2\sigma_e} = 0, \quad (7.18)$$

$$f_1 \frac{\kappa_1 - \kappa_e}{\kappa_1 + 4\mu_e/3} + f_2 \frac{\kappa_2 - \kappa_e}{\kappa_2 + 4\mu_e/3} = 0, \quad (7.19)$$

$$f_1 \frac{\mu_1 - \mu_e}{\mu_1 + \mu_e(9\kappa_e + 8\mu_e)/(6\kappa_e + 12\mu_e)} + f_2 \frac{\mu_2 - \mu_e}{\mu_2 + \mu_e(9\kappa_e + 8\mu_e)/(6\kappa_e + 12\mu_e)} = 0. \quad (7.20)$$

Milton (1984) showed that the structures that correspond to the above formulae are realized for a certain class of hierarchical granular aggregates in which grains of comparable size are well separated.

To examine our bounds for these materials, we assume that the phase properties are given by

$$\sigma_1 = 1, \quad \kappa_1 = 1, \quad \mu_1 = 1, \quad \sigma_2 = 20, \quad \kappa_2 = 10, \quad \mu_2 = 10. \quad (7.21)$$

For a fixed volume fraction, we calculate the moduli σ_e , κ_e and μ_e by solving the system of equations (7.18)–(7.20). Then we use the value σ_e to calculate the bounds on the effective bulk modulus of the composite according to theorem 1.1 and compare the bounds with the actual values κ_e . Figure 7 summarizes our findings for the bulk modulus bounds and includes the Hashin–Shtrikman bounds.

As we see, for $f_2 \leq 0.15$ or $f_2 \geq 0.95$, our cross-property bounds are tight enough to provide almost exact predictions. At intermediate volume fractions, they improve upon existing results.

The authors thank Graeme Milton for helpful discussions. We gratefully acknowledge the support of the Air Force Office of Scientific Research under Grant no. F49620-92-J-0501 and of the Department of Energy under Grant. no. DEFG02-92ER14275.

References

- Beran, M. 1968 *Statistical continuum theories*. New York: Wiley.
- Bruggeman, D. A. G. 1935 *Ann. Phys.* **24**, 636–679.
- Bruno, O. P. 1991 *Proc. R. Soc. Lond. A* **433**, 353–381.
- Bruno, O. P. & Leo, P. H. 1993 *Arch. Ration. Mech. Analysis* **121**, 303–338.
- Budiansky, B. 1965 *J. Mech. Phys. Solids* **13**, 223–227.
- Berryman, J. G. & Milton, G. W. 1988 *J. Phys. D* **21**, 87–94.
- Cherkaev, A. V. & Gibiansky, L. V. 1992 *Proc. R. Soc. Edinb. A* **122** 93–125.
- Cherkaev, A. V. & Gibiansky, L. V. 1993 *J. Mech. Phys. Solids* **41**, 937–980.
- Christensen, R. M. 1979 *Mechanics of composite materials*, New York: Wiley-Interscience.
- Dacorogna, B. 1982 *Springer Lecture Notes in Mathematics*, vol. 922. Berlin: Springer.
- Francfort, G. & Murat, F. 1986 *Arch. Ration. Mech. Analysis* **94**, 307–334.
- Gibiansky, L. V. & Lakes, R. 1993 *Mech. Mater.* **16**, 317–331.
- Gibiansky, L. V. & Milton, G. W. 1993 *Proc. R. Soc. Lond. A* **440**, 163–188.
- Gibiansky, L. V. & Torquato, S. 1993 *Phys. Rev. Lett.* **71**, 2927–2930.
- Gibiansky, L. V. & Torquato, S. 1995 *Phil. Trans. R. Soc. Lond. A* **343**, 243–274.
- Hashin, Z. 1965 *J. Mech. Phys. Solid* **13**, 119–134.
- Hashin, Z. & Shtrikman, S. 1962 *J. Appl. Phys.* **35**, 3125–3131.
- Hashin, Z. & Shtrikman, S. 1963 *J. Mech. Phys. Solids* **11**, 127–140.
- Keller, J. B., Rubinfeld, L. & Molyneux, J. 1967 *J. Fluid Mech.* **30**, 97–125.
- Kim, I. C. & Torquato, S. 1990 *J. Appl. Phys.* **69**, 2280–2289.
- Lurie, K. A. & Cherkaev, A. V. 1984 *Proc. R. Soc. Edinb. A* **99**, 71–87.
- Lurie, K. A. & Cherkaev, A. V. 1986 *Proc. R. Soc. Edinb. A* **104**, 21–38.

- Milton, G. W. 1981 *J. Appl. Phys.* **52**, 5294–5304.
- Milton, G. W. 1984 In *Physics and chemistry of porous media* (ed. D. L. Johnson & R. N. Sen). New York: American Institute of Physics.
- Milton, G. W. 1991 In *Composite media and homogenization theory* (ed. G. Dal Maso & G. Dal Antonio), (Progress in non-linear differential equations and their applications 5) (series ed. H. Brezis), pp. 223–245. Boston, MA: Birkhauser.
- Murat, F. & Tartar, L. 1985 Calcul des variations et homogénéisation, *Les Méthodes d'Homogénéisation: Théorie et Applications en Physique, Coll. de la Dir. des Etudes et Recherches d'Electr. de France, Eyrolles, Paris*, pp. 319–370.
- McKenzie, D. R., McPhedran, R. C. & Derrick, G. H. 1978 *Proc. R. Soc. Lond. A* **362**, 211–232.
- Rubinstein, J. & Keller, J. 1987 *Physics Fluids* **30**, 2919–2921.
- Rubinstein, J. & Torquato, S. 1988 *J. Chem. Phys.* **88**, 6372–6380.
- Schulgasser, K. 1976a *J. Math. Phys.* **17**, 378–381.
- Schulgasser, K. 1976b *J. Appl. Phys.* **47**, 1880–1886.
- Schulgasser, K. 1977 *Int. J. Heat Mass Transfer* **20**, 1273–1289.
- Tartar, L. 1985 In *Ennio de Giorgi Colloquium* (Pitman Research Notes in Mathematics 125) (ed. P. Kree), pp. 168–187.
- Torquato, S. 1990 *Phys. Rev. Lett.* **64**, 2644–2647.
- Torquato, S. 1992 In *Macroscopic behavior of heterogeneous materials from the microstructure* (ed. S. Torquato & D. Krajcinovic), AMD-vol. 147, pp. 53–65. New York: American Society of Mechanical Engineers.
- Torquato, S. & Rubinstein, J. 1991 *J. Appl. Phys.* **69**, 7118–7125.
- Walpole, L. J. 1966 *J. Mech. Phys. Solids* **14**, 151–162.
- Walpole, L. J. 1969 *J. Mech. Phys. Solids* **17**, 235–251.

Received 22 June 1994; accepted 28 February 1995