*J. Mech. Phys. Solids* Vol. 30, No. 5, pp. 355–376, 1982.
Printed in Great Britain.

0022-5096/82/050355-22 $03.00/0


# ELASTOSTATIC RESONANCES—A NEW APPROACH TO THE CALCULATION OF THE EFFECTIVE ELASTIC CONSTANTS OF COMPOSITES†

YACOV KANTOR and DAVID J. BERGMAN

Department of Physics and Astronomy,
Tel Aviv University, Tel Aviv 69978, Israel

(*Received* 17 *August* 1981)

ABSTRACT

A NEW method is presented for a systematic evaluation of the effective elastic tensor $C^{(e)}$ in a two-component composite. Both $C^{(e)}$ and local strain field are expanded in terms of a complete set of elastostatic resonances. The resonances are found by calculating eigenstates of a certain integral operator, and this can be carried out in stages. First one finds the eigenstates of individual, isolated grains or fibers, and only then does one attempt to calculate eigenstates of the entire composite. We apply this procedure to 2D periodic arrays of cylinders—both hexagonal and square. Using simple matrix perturbation techniques we obtain exact expansions for the elastic constants in powers of $p$, the volume fraction of the cylinders, that go up to the order $p^{11}$ in the case of bulk modulus of the hexagonal array.

## 1. INTRODUCTION

THEORIES of the effective elastic properties of composite (i.e. macroscopically inhomogeneous) systems have been applied to the calculation of the elastic properties of a variety of practically useful materials. These include polycrystalline materials as well as fibrous, fiber reinforced, and granular materials, porous rocks, etc. Various approaches to the problem have been reviewed by WATT *et al.* (1976).

In recent years, an approach that is analogous to the quantum scattering theory in solid state physics has often been used, see, e.g., ZELLER and DEDERICHS (1973), KORRINGA (1973), GUBERNATIS and KRUMHANSL (1975), KRÖNER (1977), GUBERNATIS *et al.* (1977a,b, 1979), GUBERNATIS (1979), WILLIS (1980a,b) and many others. In this approach the elastic problem (either static or dynamic) is represented in the form of an integral equation, as in the case of the scattering problem. This approach led to a reformulation and extension of various exact bounds, and also produced some approximate solutions. In this approach, one usually begins by solving the one-grain scattering problem (frequently, in the Born or long-wave approximations), and then extends this to a solution of the general problem by multiple scattering techniques. This procedure is successful when the concentration of inclusions is low, or when the elastic constants of the inclusions do not differ strongly from those of the host medium, i.e., when the scattering is weak.

† Research supported in part by the United States–Israel Binational Science Foundation under Grant No. 2006/79.

We also start from a scattering-theory-like representation of the elastostatic problem, but unlike the usual situation, our scattering operator is symmetric, though generally non-hermitian. Following a similar approach to one that was used in the electrostatic case (BERGMAN, 1979a, b) we expand the solution of the elastic problem in a set of eigenstates of the scattering operator. In this way we obtain a representation of the effective elastic constants in the form of a sum of elastostatic resonance terms, each one of which can be calculated from a knowledge of the appropriate eigenstate.

In Section 2 we develop the general theory of this approach. As an example, the results of which are used later, we find exact analytical expressions for the resonances of an infinitely long cylinder made of an isotropic elastic material embedded in an infinite isotropic medium.

A knowledge of the elastic resonances of individual, isolated grains allows us to set up the problem of finding the elastic resonances of the multi-grain system in a convenient way. This is developed in Section 3, and applied to a practical calculation of the effective elastic constants of periodic square and hexagonal arrays of cylinders in Section 4. By employing simple techniques of perturbation theory, this approach enables us to develop systematic expansions for these constants in powers of the volume fraction of the cylinders $p$. (However, we are not limited to expanding in powers of $p$!) In lowest order, we obtain in this way (different) Clausius–Mossotti-type expressions for both the bulk modulus $k$ and the shear moduli of the two systems. Some higher order corrections to these constants are also calculated—all of them by using some very simple techniques of perturbation theory. In this way, we obtain expressions for $\kappa$ correct to order $p^{11}$ and $p^7$ for hexagonal and cubic arrays, respectively. For the shear moduli we obtain expressions which are correct to order $p^5$ for both types of arrays.

## 2. THE GENERAL APPROACH

The strain tensor $\varepsilon_{kl}$ in a composite elastic medium is usually found by solving an inhomogeneous boundary value problem based on the following differential equation:

$$\partial_j \boldsymbol{C}_{ijkl}\varepsilon_{kl} = 0, \tag{2.1}$$

where $\boldsymbol{C}_{ijkl}(\mathbf{r})$ is the local elastic stiffness tensor. Note that we do not have to specify continuity conditions at the interfaces between different components—those are automatically ensured if we demand that (2.1) be satisfied even in places where $\boldsymbol{C}_{ijkl}$ has a discontinuity. However, (2.1) must be supplemented by the compatibility conditions, which connect the strain $\varepsilon_{kl}$ with the derivatives of the displacement vector $\mathbf{u}$:

$$\varepsilon_{kl} = \tfrac{1}{2}(\partial_k u_l + \partial_l u_k), \tag{2.2}$$

as well as by appropriate boundary conditions on $\mathbf{u}$. We will use homogeneous boundary conditions (see HASHIN, 1970, pp. 44–47), i.e.

$$u_i = \varepsilon^0_{ij} x_j, \quad \text{for} \quad \mathbf{r} = (x_1, x_2, x_3) \text{ on the boundary}, \tag{2.3}$$

where $\varepsilon^0_{ij}$ is some constant tensor. These boundary conditions would cause $\varepsilon_{ij}$ to be a constant equal to $\varepsilon^0_{ij}$ if the sample were homogeneous. In the case of an inhomogeneous

system, $\varepsilon_{ij}$ will usually depend on $\mathbf{r}$ in a complicated manner, but its volume average will always be equal to $\varepsilon^0_{ij}$.

The effective elastic tensor $C^{(e)}_{ijkl}$ is defined by requiring that the elastic energy density in a homogeneous sample characterized by $\boldsymbol{C}^{(e)}$ and subject to the same boundary conditions $\varepsilon^0_{ij}$ be equal to the volume average of this quantity in the real, inhomogeneous sample

$$\varepsilon^0 \boldsymbol{C}^{(e)} \varepsilon^0 = \frac{1}{V} \int \varepsilon \boldsymbol{C} \varepsilon \, \mathrm{d}V. \tag{2.4}$$

In this equation, and often also in subsequent discussions, we have suppressed the tensorial indices.

The local stiffness tensor $\boldsymbol{C}(\mathbf{r})$ of a two-component composite made of homogeneous materials with stiffness tensors $\boldsymbol{C}^{(1)}$ and $\boldsymbol{C}^{(2)}$ will be represented with the help of a step function $\theta$

$$\boldsymbol{C}(\mathbf{r}) = \boldsymbol{C}^{(2)} + \theta(\mathbf{r})(\boldsymbol{C}^{(1)} - \boldsymbol{C}^{(2)}) \equiv \boldsymbol{C}^{(2)} + \theta(\mathbf{r}) \delta \boldsymbol{C}, \tag{2.5}$$

$$\theta(\mathbf{r}) = \begin{cases} 1, \mathbf{r} \text{ inside} & \boldsymbol{C}^{(1)} \text{ material} \\ 0, \mathbf{r} \text{ outside} & \boldsymbol{C}^{(1)} \text{ material.} \end{cases} \tag{2.6}$$

We shall use a somewhat more general form of (2.5)

$$\boldsymbol{C}(\mathbf{r}) = \boldsymbol{C}^{(2)} + \frac{1}{s} \theta(\mathbf{r}) \, \delta \boldsymbol{C}. \tag{2.7}$$

By allowing $s$ to take arbitrary values, we are actually replacing the $\boldsymbol{C}^{(1)}$ material by a different material, characterized by a stiffness tensor

$$\boldsymbol{C}^{(1)'} = \boldsymbol{C}^{(2)} + \frac{1}{s} \delta \boldsymbol{C} = \frac{1}{s} \boldsymbol{C}^{(1)} + \frac{s-1}{s} \boldsymbol{C}^{(2)}. \tag{2.8}$$

By a series of transformations, including a transformation from volume to surface integration, replacement of $\varepsilon$ by $\varepsilon^0$ at the surface, and a transformation back to volume integration, we obtain from (2.4) and (2.7) the following forms for $\boldsymbol{C}^{(e)}$:

$$\varepsilon^0 \boldsymbol{C}^{(e)} \varepsilon^0 = \frac{1}{V} \int \varepsilon^0 \boldsymbol{C} \varepsilon \, \mathrm{d}V = \frac{1}{V} \int \varepsilon^0 \boldsymbol{C}^{(2)} \varepsilon \, \mathrm{d}V + \frac{1}{sV} \int \theta \varepsilon^0 \delta \boldsymbol{C} \varepsilon \, \mathrm{d}V$$

$$= \varepsilon^0 \boldsymbol{C}^{(2)} \varepsilon^0 + \frac{1}{sV} \int \theta \varepsilon^0 \delta \boldsymbol{C} \varepsilon \, \mathrm{d}V. \tag{2.9}$$

Consequently, we define the function $F(s)$ by

$$F(s) \equiv \varepsilon^0 \boldsymbol{C}^{(e)} \varepsilon^0 - \varepsilon^0 \boldsymbol{C}^{(2)} \varepsilon^0 = \frac{1}{sV} \int \theta \varepsilon^0 \delta \boldsymbol{C} \varepsilon \, \mathrm{d}V. \tag{2.10}$$

Obviously, $F(s)$ is a scalar quantity that depends on our choice of $\varepsilon^0$.

The strain tensor in a composite material is also the solution of a linear integral equation (see, e.g., WU and MCCULLOUGH, 1977), which replaces (2.1)–(2.3) and (2.7)

$$\varepsilon_{ij}(\mathbf{r}) = \varepsilon^0_{ij} + \frac{1}{s} \int \theta(\mathbf{r}) G_{ijkl}(\mathbf{r}, \mathbf{r}') \, \delta C_{klmn} \varepsilon_{mn}(\mathbf{r}') \, \mathrm{d}V'. \tag{2.11}$$

Here $\boldsymbol{G}$ is the tensor Green's function of the problem—it depends on $\boldsymbol{C}^{(2)}$ and on the shape of the sample. Note however, that $\boldsymbol{G}$ is independent of $\boldsymbol{C}^{(1)}$ and of the microgeometry of the composite. Although $\boldsymbol{G}$ is symmetric under the interchanges $i \leftrightarrow j$, $k \leftrightarrow l$ (just like $\boldsymbol{C}$), and under the joint interchange $i, j, \mathbf{r} \leftrightarrow k, l, \mathbf{r}'$, we note that the entire integral operator in (2.11) is not symmetric. We now symmetrize it with the help of the "square root tensor" of $\delta\boldsymbol{C}$, denoted by $\boldsymbol{K}_{ijkl}$

$$\boldsymbol{K}\boldsymbol{K} = \delta\boldsymbol{C}. \tag{2.12}$$

Note that $\boldsymbol{K}$ is symmetric under each of the interchanges $i \leftrightarrow j$, $k \leftrightarrow l$, $ij \leftrightarrow kl$ (just like $\delta\boldsymbol{C}$), but is not real unless $\delta\boldsymbol{C}$ is positive definite. We now define

$$\rho \equiv \boldsymbol{K}\varepsilon, \tag{2.13}$$

$$\boldsymbol{H} \equiv \boldsymbol{K}\boldsymbol{G}\boldsymbol{K}. \tag{2.14}$$

Multiplying (2.11) by $\boldsymbol{K}$ from the left we arrive at the following integral equation:

$$\rho_{ij}(\mathbf{r}) = \rho^0_{ij} + \frac{1}{s}\int \theta(\mathbf{r})\boldsymbol{H}_{ijkl}(\mathbf{r}, \mathbf{r}')\rho_{kl}(\mathbf{r}')\, \mathrm{d}V', \tag{2.15}$$

or, in a more concise symbolic bra-ket notation,

$$|\rho\rangle = |\rho^0\rangle + \frac{1}{s}\hat{H}|\rho\rangle. \tag{2.16}$$

In order to make further progress, we would like to introduce eigenstates of $\hat{H}$ and use them to expand the solution of (2.16). Such an expansion requires the definition of a scalar product between different states

$$\langle\rho|\rho'\rangle \equiv \int \theta(\mathbf{r})\rho^*_{ij}(\mathbf{r})\rho'_{ij}(\mathbf{r})\, \mathrm{d}V. \tag{2.17}$$

Note that the integration is confined to the volume of $\boldsymbol{C}^{(1)}$ material. Because the operator $\hat{H}$ is symmetric, but in general non-hermitian, under this scalar product, there exists a set of right eigenstates $|\rho^{(\alpha)}\rangle$ and a (different) set of left eigenstates $\langle\tilde{\rho}^{(\alpha)}|$ such that

$$\hat{H}|\rho^{(\alpha)}\rangle = s_\alpha|\rho^{(\alpha)}\rangle, \tag{2.18}$$

$$\langle\tilde{\rho}^{(\alpha)}|\hat{H} = \langle\tilde{\rho}^{(\alpha)}|s_\alpha. \tag{2.19}$$

The two sets satisfy the bi-orthogonality relations (see, e.g., MORSE and FESHBACH, 1953)

$$\langle\tilde{\rho}^{(\alpha)}|\rho^{(\beta)}\rangle = 0, \quad \text{for} \quad s_\alpha \neq s_\beta. \tag{2.20}$$

When there is degeneracy of eigenvalues, we can always choose the eigenstates so that they are mutually bi-orthogonal. The only property which is not automatically ensured is normalizability, i.e.,

$$\langle\tilde{\rho}^{(\alpha)}|\rho^{(\alpha)}\rangle \neq 0. \tag{2.21}$$

We will, therefore, have to assume that this property holds for all eigenstates, enabling us to normalize them to unity. This property must be verified in each particular case. It holds in the examples which are discussed in the following sections.

In many practical cases $\delta \boldsymbol{C}$ is a positive (negative) definite tensor and therefore $\boldsymbol{K}$ is a real (pure imaginary) tensor, and consequently the operator $\hat{H}$ is hermitian. Obviously, the eigenvalues $s_\alpha$ are real in those cases. In Appendix A we prove that the eigenvalues are real even in the case of non-definite $\delta \boldsymbol{C}$, i.e. non-hermitian $\hat{H}$.

By comparing (2.16) and (2.18) we can identify the physical significance of the eigenstates of $\hat{H}$. These are the elastostatic resonances of the sample, i.e., states where the sample is internally deformed and strained even though the boundaries are undeformed. Such a situation cannot occur for any physically allowed values of the elastic constants, and therefore $\boldsymbol{C}^{(1)'}$ in (2.8) must assume unphysical values for $s = s_\alpha$, i.e., it cannot be positive definite.

Using the definition of the scalar product and formally solving (2.16), we may rewrite (2.10) in the following form:

$$F(s) = \frac{1}{sV}\langle \rho^{0*} | \rho \rangle = \frac{1}{V}\langle \rho^{0*} \left| \frac{1}{s - \hat{H}} \right| \rho^0 \rangle. \tag{2.22}$$

Note that the left hand state in this equation is the complex conjugate of $\rho^0$, namely

$$|\rho^{0*}\rangle = \boldsymbol{K}^* \varepsilon^{0*}. \tag{2.23}$$

We now use the bi-orthogonal set (assumed to be a complete set) of eigenstates of $\hat{H}$ in order to write the following expansion for the identity operator

$$\hat{I} = \sum_\alpha |\rho^{(\alpha)}\rangle \langle \tilde{\rho}^{(\alpha)}|. \tag{2.24}$$

Using this operator we can bring (2.22) to the following form:

$$F(s) = \sum_\alpha \frac{F_\alpha}{s - s_\alpha} \tag{2.25}$$

where

$$F_\alpha \equiv \frac{1}{V}\langle \rho^{0*} | \rho^{(\alpha)} \rangle \langle \tilde{\rho}^{(\alpha)} | \rho^0 \rangle. \tag{2.26}$$

In Appendix A we prove that the weights $F_\alpha$ are real, and that the product $F_\alpha \cdot s_\alpha$ is always negative (in the degenerate case, $F_\alpha$ must be replaced in this product by the sum of all $F_\alpha$ corresponding to the same value of $s_\alpha$). By analogy with the electrostatic problem in a composite material (BERGMAN and KANTOR, 1981), we believe that the pole spectrum in (2.25) is discrete as long as all the internal interfaces between different components are smooth surfaces (i.e., no corners or contact points). To the best of our knowledge, a rigorous proof of this conjecture exists only for the case when the two materials are both isotropic and have equal Poisson ratios (KUPRADZE, 1965).

## 3. ISOLATED CYLINDRICAL INCLUSION

In this section we discuss the problem of a single infinitely long cylinder, with radius $R$ and stiffness tensor $\boldsymbol{C}^{(1)}$, embedded in an infinite medium with elastic tensor $\boldsymbol{C}^{(2)}$. Both $\boldsymbol{C}^{(1)}$ and $\boldsymbol{C}^{(2)}$ are assumed to be isotropic. We shall concentrate on the two-dimensional (2D) elastic problem in the plane perpendicular to the cylinder axis. Adding the third direction is a trivial matter. The stiffness tensor in a 2D isotropic material has the form

$$\boldsymbol{C}^{(1,2)}_{ijkl} = \lambda^{(1,2)}\delta_{ij}\delta_{kl} + 2\mu^{(1,2)}\boldsymbol{I}_{ijkl} \tag{3.1}$$

where

$$\boldsymbol{I}_{ijkl} = \tfrac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{3.2}$$

and where the subscripts stand for *two* orthogonal directions in the plane. If we are discussing the plane strain problem, where the $u_3$ component of the displacement vector $\mathbf{u}$ vanishes, then the Lamé constants $\lambda$ and $\mu$ are the same as the usual three-dimensional constants. However, when we discuss the plane stress situation, where the $\sigma_{13}, \sigma_{23}, \sigma_{33}$ components of the stress tensor vanish, then $\lambda$ must be replaced by $2\lambda\mu/(\lambda + 2\mu)$ (see, e.g., SOKOLNIKOFF, 1956, pp. 250–257). The 2D shear modulus is equal to $\mu$, while the 2D bulk modulus is given by $\kappa = \lambda + \mu$.

In what follows we will discuss, among others, systems with square symmetry. Such systems are characterized by three independent elastic constants, which we shall choose as follows:

$$\kappa \equiv \tfrac{1}{4}(\boldsymbol{C}_{1111} + \boldsymbol{C}_{2222} + 2\boldsymbol{C}_{1122}), \tag{3.3a}$$

$$\mu \equiv \boldsymbol{C}_{1212}, \tag{3.3b}$$

$$M \equiv \tfrac{1}{4}(\boldsymbol{C}_{1111} + \boldsymbol{C}_{2222} - 2\boldsymbol{C}_{1122}). \tag{3.3c}$$

The additional shear modulus $M$ coincides with $\mu$ for an isotropic system.

It is convenient to represent both components of the 2D displacement vector $\mathbf{u}(x_1, x_2)$ as functions of the complex variable $z = x_1 + ix_2$. A detailed calculation of the elastostatic resonances is given in Appendix B—only the final results are presented here.

As we explained in Section 2, the eigenstates can occur only for special, non-physical values of $\boldsymbol{C}^{(1)'}$. In the isotropic case, $\boldsymbol{C}^{(1)'}$ is completely characterized by the bulk modulus $\kappa^{(1)'}$ and the shear modulus $\mu^{(1)'}$ of cylindrical material. The resonant values of these parameters lie upon four curves in the $\kappa^{(1)'}, \mu^{(1)'}$ plane, as shown in Fig. 1. Note that there are no resonances in the physical part of the plane, where $\kappa^{(1)'}$ and $\mu^{(1)'}$ are both positive.

As we vary $s$, (2.8) constrains $\kappa^{(1)'}$ and $\mu^{(1)'}$ to move along a straight line in that plane. The eigenvalues $s_\alpha$ are determined by the intersection of that line with the four curves of Fig. 1. Consequently, there are at most four different eigenvalues, and correspondingly a high degree of degeneracy.

The vertical line in Fig. 1 (denoted by A) is described by

$$\kappa^{(1)'} = -\mu^{(2)}. \tag{3.4}$$

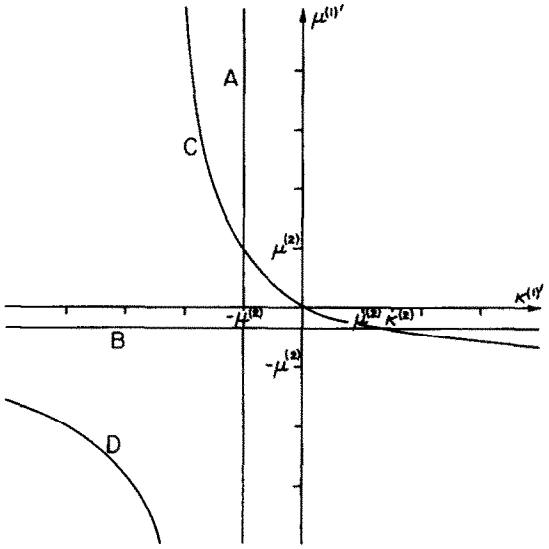


FIG. 1. Location of the resonance values $\kappa^{(1)'}$ and $\mu^{(1)'}$ of the cylinder material in the $\kappa, \mu$ plane. The curves are defined by (3.4) (line A), (3.7) (line B), (3.10) (hyperbola branches C and D). In order to draw this set of curves, we assumed the particular relationship $\kappa^{(2)} = 1.5\mu^{(2)}$, but otherwise the values of $\kappa^{(1)}$, $\kappa^{(2)}$, $\mu^{(1)}$, $\mu^{(2)}$ are arbitrary.

The corresponding eigenvalue is

$$s_A = -\frac{\delta\kappa}{\mu^{(2)}+\kappa^{(2)}}, \tag{3.5}$$

and the right eigenstate is

$$\rho^{(A0)} = \begin{pmatrix} \rho_{11}^{(A0)} \\ \rho_{22}^{(A0)} \\ \rho_{12}^{(A0)} \end{pmatrix} = \begin{cases} \dfrac{1}{\sqrt{(2\pi)R}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} & , \text{ for } |z| \leqslant R \\ \dfrac{R}{\sqrt{(2\pi)}} \left(\dfrac{\delta\mu}{\delta\kappa}\right)^{1/2} \mathrm{Re}\begin{pmatrix} -1 \\ 1 \\ -\mathrm{i} \end{pmatrix} \dfrac{1}{z^2} & , \text{ for } |z| > R. \end{cases} \tag{3.6}$$

(The superscript 0 signifies the fact that this is also an eigenstate of angular momentum $\hat{J}$ with eigenvalue $m = 0$, see Appendix B). The corresponding left eigenstate is created by replacing $(\delta\mu/\delta\kappa)^{1/2}$ in (3.6) by its complex conjugate. The displacement vector field **u** of this eigenstate is depicted in Fig. 2(a). Inside the cylinder it corresponds to a pure, uniform compression, while outside it is proportional to $1/|z|$. We call this state a "compression dipole".

The horizontal line in Fig. 1 (denoted by B) is described by

$$\mu^{(1)'} = -\frac{\mu^{(2)}\kappa^{(2)}}{\kappa^{(2)}+2\mu^{(2)}}, \tag{3.7}$$

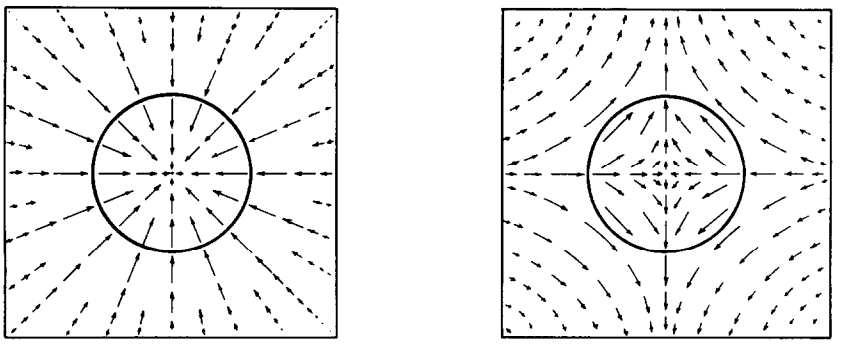


FIG. 2. The displacement vector field **u** of (a) the compression-dipole and (b) one of the shear-dipole resonance states (the other one has the same form, but rotated by an angle $\pi/4$).

and the corresponding eigenvalue is

$$s_{\mathrm{B}} = -\frac{\delta\mu(\kappa^{(2)}+2\mu^{(2)})}{2\mu^{(2)}(\kappa^{(2)}+\mu^{(2)})}. \tag{3.8}$$

There are infinitely many right eigenstates corresponding to this eigenvalue:

$$\rho^{(\pm \mathrm{B}m)} = \begin{cases} A_{\mathrm{B}m} \begin{Bmatrix} \mathrm{Re} \\ \mathrm{Im} \end{Bmatrix} \begin{pmatrix} -1 \\ 1 \\ -\mathrm{i} \end{pmatrix} z^{m-2} & , \text{ for } |z| \leqslant R, \\ A_{\mathrm{B}m} \dfrac{R^{2(m-1)}\kappa^{(2)}}{\kappa^{(2)}+2\mu^{(2)}} \left[ \dfrac{2\mu^{(2)}}{\kappa^{(2)}} \left( \dfrac{\delta\kappa}{\delta\mu} \right)^{1/2} \begin{Bmatrix} \mathrm{Re} \\ \mathrm{Im} \end{Bmatrix} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \dfrac{1}{z^{*m}} \right. & \\ \left. + \begin{Bmatrix} \mathrm{Re} \\ \mathrm{Im} \end{Bmatrix} \begin{pmatrix} 1 \\ -1 \\ \mathrm{i} \end{pmatrix} \left[ \dfrac{mz}{z^{*m+1}} - \dfrac{(m+1)R^2}{z^{*m+2}} \right] \right] & , \text{ for } |z| > R, \end{cases} \tag{3.9a}$$

$$A_{\mathrm{B}m} \equiv \left( \frac{m-1}{2\pi} \right)^{1/2} \frac{1}{R^{m-1}} \tag{3.9b}$$

where $m = 2, 3, \ldots$, and where $(\pm)$ corresponds to $\begin{Bmatrix} \mathrm{Re} \\ \mathrm{Im} \end{Bmatrix}$ on the r.h.s. Each of these states is also an eigenstate of $\hat{J}^2$, with an eigenvalue equal to $m^2$, and an eigenstate of the reflection operator through the $x_1$-axis with the eigenvalue $\pm 1$. The left eigenstates are obtained by replacing $\sqrt{(\delta\kappa/\delta\mu)}$ by its complex conjugate in (3.9a). The **u**-field of the $\rho^{(+\mathrm{B}2)}$ state is depicted in Fig. 2(b). The **u**-field of $\rho^{(-\mathrm{B}2)}$ is given by the same figure but rotated by $\pi/4$. Inside the cylinder these two states correspond to a pure, uniform shear,

while outside it they decrease asymptotically like $1/|z|$. We will call these states (first and second) "shear dipoles".

The curved lines in Fig. 1 (denoted by C, D) are the two branches of a hyperbola described by the following equation:

$$\frac{\mu^{(1)'}\kappa^{(1)'}}{\kappa^{(1)'}+2\mu^{(1)'}} = -\mu^{(2)}. \tag{3.10}$$

From these curves, two different eigenvalues are found for $s$, determined by the following quadratic equation:

$$s_{C,D}^2 2\mu^{(2)}(\mu^{(2)}+\kappa^{(2)}) + s_{C,D}[2\mu^{(2)}\delta\kappa + (\kappa^{(2)}+2\mu^{(2)})\delta\mu] + \delta\mu\delta\kappa = 0 \tag{3.11}$$

and they are both infinitely degenerate. The right eigenstates are

$$\rho^{(\pm C,Dm)} = \begin{cases} A_{C,Dm}\left[\dfrac{2\mu_{C,D}^{(1)'}}{\kappa_{C,D}^{(1)'}}\left(\dfrac{\delta\kappa}{\delta\mu}\right)^{1/2}\begin{Bmatrix}\mathrm{Re}\\ \mathrm{Im}\end{Bmatrix}\begin{pmatrix}1\\ 1\\ 0\end{pmatrix} z^m \right. \\ \qquad \left. + \begin{Bmatrix}\mathrm{Re}\\ \mathrm{Im}\end{Bmatrix}\begin{pmatrix}-1\\ 1\\ -\mathrm{i}\end{pmatrix}[mz^* z^{m-1} - (m-1)R^2 z^{m-2}]\right], \quad \text{for} \quad |z| \leqslant R \\ A_{C,Dm} R^{2(m+1)} \dfrac{\mu_{C,D}^{(1)'}}{\mu^{(2)}} \begin{Bmatrix}\mathrm{Re}\\ \mathrm{Im}\end{Bmatrix}\begin{pmatrix}1\\ -1\\ -\mathrm{i}\end{pmatrix}\dfrac{1}{z^{*m+2}}, \quad , \quad \text{for} \quad |z| > R \end{cases} \tag{3.12a}$$

$$A_{C,Dm} \equiv \left(\frac{m+1}{\pi\left[\dfrac{\delta\kappa}{\delta\mu}(2\mu_{C,D}^{(1)'}/\kappa_{C,D}^{(1)'})^2 + 2\right]}\right)^{1/2} \frac{1}{R^{m+1}} \tag{3.12b}$$

where $m = 1, 2, \ldots$, and where $\mu_{C,D}^{(1)'}$ and $\kappa_{C,D}^{(1)'}$ are the values of $\mu^{(1)'}$ and $\kappa^{(1)'}$ for $s = s_{C,D}$. The superscripts $m$ and $(\pm)$ have the same meaning as for the B-type states. The left eigenstates are obtained by replacing $A_{C,Dm}$ and $(\delta\kappa/\delta\mu)^{1/2}$ in (3.12a) by their complex conjugates. Outside the cylinder all of these states decrease with distance faster than the dipolar states $\rho^{(A0)}$ and $\rho^{(\pm B2)}$.

Different choices of $\varepsilon^0$ (and hence $\rho^0$) enable us to isolate different parts of the tensor $\boldsymbol{C}^{(e)}$ [see (2.10)]. In what follows we shall use the following choices of $\varepsilon^0$:

$$\varepsilon_{ij}^{0\kappa} = \tfrac{1}{2}\delta_{ij}, \qquad \rho_{ij}^{0\kappa} = \left(\frac{\delta\kappa}{2}\right)^{1/2}\delta_{ij}, \tag{3.13a}$$

$$\varepsilon_{ij}^{0\mu} = \boldsymbol{I}_{ij12}, \qquad \rho_{ij}^{0\mu} = (2\delta\mu)^{1/2}\boldsymbol{I}_{ij12}, \tag{3.13b}$$

$$\varepsilon_{ij}^{0M} = \tfrac{1}{2}(\boldsymbol{I}_{ij11} - \boldsymbol{I}_{ij22}), \qquad \rho_{ij}^{0M} = \left(\frac{\delta\mu}{2}\right)^{1/2}(\boldsymbol{I}_{ij11} - \boldsymbol{I}_{ij22}). \tag{3.13c}$$

The expressions for $\rho^0$ follow from (2.13) and from the $\boldsymbol{K}$ tensor given in (B.5). The choices (3.13a–c) select the coefficients $\kappa$, $\mu$, $M$, defined by (3.3a–c), respectively. The

only non-vanishing scalar products that will appear in (2.26) will be $\langle\tilde{\rho}^{(A0)}|\rho^{0\kappa}\rangle$, $\langle\tilde{\rho}^{(+B2)}|\rho^{0\mu}\rangle$ and $\langle\tilde{\rho}^{(-B2)}|\rho^{0M}\rangle$.

Using these results, we can easily write down the effective elastic constants for a composite that has just one cylindrical inclusion. Of course, in the limit of an infinite volume for the host material, the effective constants approach those of the host. Therefore we are really interested in the corrections of order $1/V$ for a very large volume of the system. To order $1/V$ we thus find that there is only one non-zero term in (2.25). Choosing $\rho^0 = \rho^{0\kappa}$, we get

$$F(s) = \frac{1}{S}\frac{\langle\rho^{0\kappa *}|\rho^{(A0)}\rangle\langle\tilde{\rho}^{(A0)}|\rho^{0\kappa}\rangle}{s - s_A} = \frac{1}{S}\frac{\pi R^2\delta\kappa}{s + \delta\kappa/(\kappa^{(2)} + 2\mu^{(2)})} \tag{3.14}$$

where $S$ is the total area of the 2D sample. Taking $s = 1$ and nothing that the volume fraction is given by $p = \pi R^2/S$, we finally get

$$\kappa^{(e)} = \kappa^{(2)} + \frac{p}{(1/\delta\kappa) + [1/(\kappa^{(2)} + \mu^{(2)})]}. \tag{3.15}$$

Similarly, taking $\rho^0 = \rho^{0\mu}$ we get

$$\mu^{(e)} = \mu^{(2)} + \frac{p}{(1/\delta\mu) + \{(\kappa^{(2)} + 2\mu^{(2)})/[2\mu^{(2)}(\kappa^{(2)} + \mu^{(2)})]\}}. \tag{3.16}$$

It is obvious that $M^{(e)} = \mu^{(e)}$ in this case, and this can also be verified by a direct calculation with $\rho^0 = \rho^{0M}$. Equations (3.15) and (3.16) can also be derived by considering one cylindrical inclusion in a uniform external strain field (ESHELBY, 1957).

## 4. A System of Many Inclusions

It is convenient to set up the problem of many inclusions of one elastic material embedded in another elastic medium in terms of the eigenstates of the isolated inclusions. In our discussion of this, we follow a similar discussion given by BERGMAN (1979a, b) for the electrostatic problem of many inclusions.

For a system consisting of many non-overlapping inclusions we can write the $\theta$-function, which was defined in (2.6), as a sum of $\theta$-functions of individual grains:

$$\theta = \sum_a \theta_a \tag{4.1}$$

where $a$ is a grain index. Similarly, the operator $\hat{H}$ can be written as a sum of individual grain operators [see (2.15)]

$$\hat{H} = \sum_a \hat{H}_a. \tag{4.2}$$

Each isolated grain has its own set of eigenvalues and of right eigenstates

$$\hat{H}_a|\rho^{a(\alpha)}\rangle = s_{a\alpha}|\rho^{a(\alpha)}\rangle \tag{4.3}$$

and a similar equation for the left eigenstates. Assuming that $\{\rho^{a(\alpha)}\}$ is a complete set of

eigenstates inside the $a$th grain, we use these states to expand any eigenstate $\rho^{(r)}$ of the entire system inside the grains

$$\theta|\rho^{(r)}\rangle = \sum_{a\alpha} \mathrm{B}^{(r)}_{a\alpha}\theta_a|\rho^{a(\alpha)}\rangle. \tag{4.4}$$

The various $\theta$-functions have to appear in this equation because the states $\rho^{a(\alpha)}$ for a given $a$ form a complete set of states only inside the grain $a$. We now use this expansion in order to rewrite (2.18) as a matrix equation for the expansion coefficients $\mathrm{B}^{(r)}_{a\alpha}$. The resulting equation is

$$(s_r - s_{b\beta})\mathrm{B}^{(r)}_{b\beta} = \sum_{\substack{a\alpha \\ a\neq b}} \langle\tilde{\rho}^{b(\beta)}|\theta_b\hat{H}\theta_a|\rho^{a(\alpha)}\rangle \mathrm{B}^{(r)}_{a\alpha} \tag{4.5}$$

where $s_r$ is the eigenvalue of $\rho^{(r)}$.

The matrix element appearing on the r.h.s. can be written explicitly in terms of an overlap integral between the individual grain states $\tilde{\rho}^{b(\beta)}$ and $\rho^{a(\alpha)}$ as follows:

$$\langle\tilde{\rho}^{b(\beta)}|\theta_b\hat{H}\theta_a|\rho^{a(\alpha)}\rangle = s_{a\alpha}\langle\tilde{\rho}^{b(\beta)}|\theta_b|\rho^{a(\alpha)}\rangle = s_{a\alpha}\int \theta_b\tilde{\rho}^{b(\beta)*}\rho^{a(\alpha)}\,\mathrm{d}V, \quad \text{for} \quad b\neq a. \tag{4.6}$$

Note that the integrand includes summation over the tensorial indices of $\rho$, and that the integration is only over the volume of grain $b$. This matrix is hermitian if the operator $\hat{H}$ is hermitian.

Having found the normalized right and left eigenvectors $\mathrm{B}^{(r)}_{b\beta}$, $\tilde{\mathrm{B}}^{(r)}_{b\beta}$ as well as the eigenvalues $s_r$ of (4.5), we can again use (2.25) for $F(s)$, with the weights now being expressed as follows:

$$F_r = \frac{1}{V}\left(\sum_{a\alpha} \mathrm{B}^{(r)}_{a\alpha}\langle\rho^{0*}|\rho^{a(\alpha)}\rangle\right)\left(\sum_{a\alpha} \tilde{\mathrm{B}}^{(r)}_{a\alpha}\langle\tilde{\rho}^{a(\alpha)}|\rho^{0}\rangle\right). \tag{4.7}$$

In the hermitian case, the two factors in round brackets are complex conjugates of each other up to a sign change. Since the overlap integrals decrease with the distance between two grains, to leading order in $p$ (i.e., to order $p^0$) we can neglect the r.h.s. of (4.5). In that order, the eigenstates are equal to the individual grain eigenstates. That is why (3.15) and (3.16), if used for any system of parallel cylindrical fibers, are correct to order $p^1$.

In attempting to calculate more accurate results, a great simplification occurs if the inclusions are all identical, and form a periodic array in space. Clearly in that case the matrix element of (4.6) depends on the two grain indices $a$ and $b$ only through their vector separation $\mathbf{a}-\mathbf{b}$, and the individual grain eigenvalues $s_{a\alpha} = s_\alpha$ are independent of $a$. In that case, Bloch's theorem immediately specifies the dependence of the eigenvectors on the grain index $a$

$$\mathrm{B}^{(r)}_{a\alpha} = \frac{1}{\sqrt{N}}\mathrm{B}^{(r)}_{\alpha}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{a}}. \tag{4.8}$$

Furthermore, since $\rho^0$ is independent of $\mathbf{r}$ while $\rho^{a(\alpha)}$ is a function only of $\mathbf{r}-\mathbf{a}$, the scalar products $\langle\rho^{0*}|\rho^{a(\alpha)}\rangle$ and $\langle\tilde{\rho}^{a(\alpha)}|\rho^0\rangle$ are independent of $a$. Consequently, (4.7) simplifies to

$$F_r = \frac{N}{V}\delta_{\mathbf{k},0}\left(\sum_{\alpha} \mathrm{B}^{(r)}_{\alpha}(\mathbf{k}=0)\langle\rho^{0*}|\rho^{a(\alpha)}\rangle\right)\left(\sum_{\alpha} \tilde{\mathrm{B}}^{(r)}_{\alpha}(\mathbf{k}=0)\langle\tilde{\rho}^{a(\alpha)}|\rho^{0}\rangle\right) \tag{4.9}$$

where there is no longer any summation over grain indices. We see that only the $\mathbf{k} = 0$ Bloch states can have non-zero weights, so that only those states need to be considered. For the $\mathbf{k} = 0$ eigenstates (4.5) becomes

$$(s_r - s_\beta)\mathbf{B}_\beta^{(r)} = \sum_\alpha Q_{\beta\alpha}\mathbf{B}_\alpha^{(r)} \tag{4.10}$$

where

$$Q_{\beta\alpha} \equiv \sum_{\substack{a \\ a \neq b}} \langle \tilde{\rho}^{b(\beta)} | \theta_b \hat{H} \theta_a | \rho^{a(\alpha)} \rangle. \tag{4.11}$$

At this point it might be worthwhile to note the similarity of this approach to the tight-binding method for calculating the quantum-mechanical states of an electron in a crystal lattice. In principle, we could get a continuous band of eigenvalues $s_r(\mathbf{k})$, but only the $\mathbf{k} = 0$ state turns out to be important.

## 5. PERIODIC ARRAY OF CYLINDERS

We now apply the methods developed in the previous section to a calculation of the effective elastic constants of a composite in the form of a periodic array of parallel, identical, non-overlapping cylindrical inclusions. Both the inclusions and the host are taken to be isotropic, and we consider both hexagonal and square arrays. The individual grain eigenstates were calculated in Section 3 and Appendix B. The overlap integrals are listed in Appendix C. We still have to evaluate sums over matrix elements in order to get the $Q_{\beta\alpha}$ of (4.11). This will involve summation of terms such as $1/z^m$ or $|z|^2/z^m$ over all the points of an hexagonal or square plane lattice, a task which will usually have to be accomplished numerically.

A special problem arises in the summation of overlap integrals between two dipole states: there appears a lattice sum of terms of the form $|z|^2/z^4$, which is only semi-convergent, for which the distant contributions are just as important as the nearby ones. However, the states of grains that are near the surface of the system are not accurately given by the results of Section 3, where we assumed that the isolated cylinder was infinitely far away from the surface. Therefore, we can only use the overlap integrals of Appendix C to sum over the nearby lattice sites, and we must resort to a different stratagem for dealing with the distant contributions. For example, the overlap between two $\rho^{(A0)}$ states (compressional dipoles) of different cylinders always vanishes. Nevertheless, we shall see that the sum of such interactions between all pairs of cylinders is nonzero: this is caused by the deviation from the infinite volume expressions as one of the cylinders approaches the surface of the system. Problems arising from semi-convergence of dipole–dipole interactions are well known, and have been discussed quite extensively in recent years in the context of elasticity and fluid mechanics (see, e.g., BATCHELOR, 1974; JEFFREY, 1974; WILLIS and ACTON, 1976).

It seems, however, that the analogous problem in electrostatics was already solved at the beginning of this century by means of the concept of the local Lorentz field (cf. ASHCROFT and MERMIN, 1976; BERGMAN, 1979a, b). In Appendix D we show how to

treat these semi-convergent sums conveniently in our case. According to (D.7), if $\beta$ and $\alpha$ are any of the dipolar states (i.e., either compressional or shear), then

$$Q_{\beta\alpha} = \lim_{L\to\infty} \sum_{\substack{a \\ 0\neq|\mathbf{b}-\mathbf{a}|<L}} \langle \tilde{\rho}^{b(\beta)}|\theta_b \hat{H} \theta_a|\rho^{a(\alpha)}\rangle - s_\alpha p \delta_{\alpha\beta} \tag{5.1}$$

where the summation is performed over all the lattice points that lie on the inside of a circle of radius $L$, which is afterwards increased to infinity.

If both states are compression dipoles $p^{(A0)}$ then, as we mentioned before all terms of that sum vanish and we find

$$Q_{A0,A0} = -ps_A. \tag{5.2}$$

The values of the other $Q$'s already depend on the point symmetry of the lattice. If the lattice is invariant under reflection through the $x_1$-axis, then

$$Q_{A0,+B2} = Q_{A0,-B2} = Q_{+B2,-B2} = Q_{-B2,+B2} = 0. \tag{5.3}$$

This can easily be concluded from the expressions for the overlap integrals in Appendix C.

In the case of a hexagonal lattice we find for the remaining dipolar $Q$'s that the lattice sums over a finite circle vanish, and we are left with

$$Q_{+B2,+B2} = Q_{-B2,-B2} = -ps_B. \tag{5.4}$$

Thus, taking into account only the strongest (dipole–dipole) interactions, the secular equation (4.10) for the hexagonal lattice is already in diagonal form:

$$\begin{pmatrix} s_A(1-p) & 0 & 0 \\ 0 & s_B(1-p) & 0 \\ 0 & 0 & s_B(1-p) \end{pmatrix} \begin{pmatrix} B^{(r)}_{A0} \\ B^{(r)}_{+B2} \\ B^{(r)}_{-B2} \end{pmatrix} = s_r \begin{pmatrix} B^{(r)}_{A0} \\ B^{(r)}_{+B2} \\ B^{(r)}_{-B2} \end{pmatrix}. \tag{5.5}$$

The same equations hold also for $\tilde{\mathbf{B}}_\alpha$. The effective elastic constants will have a similar form to those of a single cylinder [see (3.15) and (3.16)] but with shifted poles

$$\kappa^{(e)} = \kappa^{(2)} + \frac{p}{(1/\delta\kappa) + [(1-p)/(\kappa^{(2)} + \mu^{(2)})]}, \tag{5.6}$$

$$\mu^{(e)} = M^{(e)} = \mu^{(2)} + \frac{p}{(1/\delta\mu) + \{(1-p)(\kappa^{(2)} + 2\mu^{(2)})/[2\mu^{(2)}(\kappa^{(2)} + \mu^{(2)})]\}}. \tag{5.7}$$

These results are equivalent to the well-known expressions for the Hashin–Shtrikman bounds on $\kappa^{(e)}$ and $\mu^{(e)}$ for transversely isotropic composite materials (HASHIN, 1970, pp. 250–274). An identical expression for $\kappa^{(e)}$ was obtained by HASHIN and ROSEN (1964) as an exact result for a composite made entirely of parallel, two component, coated circular cylinders of different sizes but with identical volume ratios. Identical expressions for both $\kappa^{(e)}$ and $\mu^{(e)}$ can be obtained for dilute isotropic suspensions in 2D, i.e. aligned cylindrical inclusions (see ESHELBY, 1957; HILL, 1965 and WALPOLE, 1969, 1972). These expressions are the elastostatic analogs of the Clausius–Mossotti or Maxwell–Garnett approximation in electrostatics.

In the case of a square lattice, the remaining dipolar $Q$'s involve lattice sums that do

not vanish. Consequently, we find

$$Q_{\pm B2,\pm B2}=\left[\pm\frac{1}{1+(2\mu^{(2)}/\kappa^{(2)})}\lim_{L\to\infty}\mathrm{Re}\left(6R^4\sum_{\substack{z\\0<|z|<L}}\frac{1}{z^4}-2R^2\sum_{\substack{z\\0<|z|<L}}\frac{|z|^2}{z^4}\right)-p\right]s_B$$
$$=\left(\pm\frac{1.92p^2-1.60p}{1+(2\mu^{(2)})/(\kappa^{(2)})}-p\right)s_B. \quad (5.8)$$

Note that the value of the semi-convergent sum of terms $|z|^2/z^4$ (equal to 2.5076... in units of the lattice constant) depends crucially on the particular type of summation (i.e., all the points inside a circle). The secular equation in this case is

$$\begin{pmatrix} s_A(1-p) & 0 & 0 \\ 0 & s_B\left(1-p-\dfrac{1.60p-1.92p^2}{1+(2\mu^{(2)}/\kappa^{(2)})}\right) & 0 \\ 0 & 0 & s_B\left(1-p+\dfrac{1.60p-1.92p^2}{1+(2\mu^{(2)}/\kappa^{(2)})}\right) \end{pmatrix}\begin{pmatrix} B^{(r)}_{A0} \\ B^{(r)}_{+B2} \\ B^{(r)}_{-B2} \end{pmatrix}$$
$$=s_r\begin{pmatrix} B^{(r)}_{A0} \\ B^{(r)}_{+B2} \\ B^{(r)}_{-B2} \end{pmatrix} \quad (5.9)$$

and the same for $\tilde{B}^{(r)}_{\alpha}$.

The effective bulk modulus is thus the same as in the hexagonal lattice, but the shear moduli are different

$$\mu^{(e)}=\mu^{(2)}+\frac{p}{(1/\delta\mu)+(1-p)(\kappa^{(2)}+2\mu^{(2)})/[2\mu^{(2)}(\kappa^{(2)}+\mu^{(2)})]+[\kappa^{(2)}(1.60p-1.92p^2)]/(\kappa^{(2)}+\mu^{(2)})}, \quad (5.10)$$

$$M^{(e)}=\mu^{(2)}+\frac{p}{(1/\delta\mu)+(1-p)(\kappa^{(2)}+2\mu^{(2)})/[2\mu^{(2)}(\kappa^{(2)}+\mu^{(2)}]-[\kappa^{(2)}(1.60p-1.92p^2)]/(\kappa^{(2)}+\mu^{(2)})}. \quad (5.11)$$

Note that (5.10), (5.11) and (5.7) begin to differ already at order $p^2$.

The order of the secular matrix, and with it the accuracy of the result, can easily be increased: Although $Q$ is an infinite matrix, it is clear that the elements which connect higher $m$ states are of higher and higher order in $p$. Therefore, when we truncate the matrix at some finite order $m$, we actually get a result which is correct to some finite order in $p$. Furthermore, many of the matrix elements vanish because (a) overlap integrals between some types of states vanish (due to the cylindrical symmetry of

individual grains), (b) many sums vanish because of the lattice symmetry, e.g. $Q_{A0,+Bm}$ vanishes for a hexagonal (square) lattice unless $m$ is an integral multiple of 6(4).

This allows us to obtain the elastic constants, to a rather high order in $p$, very easily. For instance, if we wish to improve the expression for $\kappa^{(e)}$ in an hexagonal lattice, taking it up to order $p^{11}$, we only need to diagonalize the following $2 \times 2$ matrix:

$$\begin{pmatrix} s_A(1-p) & -0.275\dfrac{\sqrt{(\delta\kappa\,\delta\mu)}}{\kappa^{(2)}+\mu^{(2)}}p^3 \\ -0.275\dfrac{\sqrt{(\delta\kappa\,\delta\mu)}}{\kappa^{(2)}+\mu^{(2)}}p^3 & s_B+\dfrac{\delta\mu\kappa^{(2)}(6.05p^5-6.09p^6)}{\mu^{(2)}(\kappa^{(2)}+\mu^{(2)})} \end{pmatrix} \begin{pmatrix} B^{(r)}_{A0} \\ B^{(r)}_{+B6} \end{pmatrix} = s_r \begin{pmatrix} B^{(r)}_{A0} \\ B^{(r)}_{+B6} \end{pmatrix}. \tag{5.12}$$

It can be shown that all other elements of the secular equation do not influence the state $\rho^{(A0)}$ to that order. A similar calculation performed for the square lattice yields a result that is correct to order $p^7$. The bulk moduli for the two cases are then given by the following expressions:

$$\kappa^{(e)} = {}^{(2)} + p\delta\kappa\left[\frac{1-G/(s'_A-s_B)^2}{1-s'_A-G/(s'_A-s_B)} + \frac{G/(s'_A-s_B)^2}{1-s_B}\right], \tag{5.13a}$$

$$s'_A = s_A(1-p), \tag{5.13b}$$

$$G = 0.0754\frac{\delta\kappa\,\delta\mu}{(\kappa^{(2)}+\mu^{(2)})^2}p^6, \quad \text{for the hexagonal lattice,} \tag{5.13c}$$

$$G = 0.306\frac{\delta\kappa\,\delta\mu}{(\kappa^{(2)}+\mu^{(2)})^2}p^4, \quad \text{for the square lattice.} \tag{5.13d}$$

From these equations, we see that the corrections to the previous result (5.6) begin with order $p^7$ ($p^5$) for the hexagonal (square) lattice. This enables us to understand why (5.6) gives such excellent agreement with more precise numerical calculations of $\kappa^{(e)}$ over a wide range of values of $p$ in the case of hexagonal lattice, as noted by HASHIN (1970, p. 179).

Similarly, we can extend the results for the shear moduli to higher order in $p$. For instance, in the case of the hexagonal lattice, by diagonalizing a $2 \times 2$ matrix we can obtain $\mu^{(e)}$ correctly to order $p^5$:

$$\mu^{(e)} = \mu^{(2)} + p\delta\mu\left[\frac{1-G/(s_Bp)+[G/(s_Bp)]^2}{1-s_B(1-p)+G/(s_Bp)} + \frac{G/(s_Bp)^2[1-G/(s_Bp)^2]}{1-s_B}\right], \tag{5.14a}$$

$$G = \left[\frac{\delta\mu\kappa^{(2)}}{(\kappa^{(2)}+\mu^{(2)})\mu^{(2)}}(2.11p^2-2.26p^3)\right]^2. \tag{5.14b}$$

Comparing this result with (5.7) we find that the corrections begin with order $p^4$. Again, this explains the good agreement between precise numerical results and (5.7) that was noted by HASHIN (1970, pp. 294–296).

In the case of the square lattice the deviation of $\mu^{(e)}$ and $M^{(e)}$ from (5.10) and (5.11) starts with order $p^5$. Oddly enough, these corrections begin at higher order than in the case of the hexagonal lattice. In this case a $4 \times 4$ matrix must be treated in order to

obtain the corrections of order $p^5$. The shear modulus of the square lattice is given by

$$\mu^{(e)} = \mu^{(2)} + p\delta\mu\left[\frac{1-G/A^2-R_C/(s_B-s_C)^2-R_D/(s_B-s_D)^2}{1-s_B-A-R_C/(s_B-s_C)-R_D(s_B-s_D)}\right.$$
$$\left.+\frac{G/A^2}{1-s_B}+\frac{R_C/(s_C-s_D)^2}{1-s_C}+\frac{R_D/(s_D-s_B)^2}{1-s_D}\right], \quad (5.15a)$$

$$G=\left[\frac{\delta\mu\kappa^{(2)}}{2\mu^{(2)}(\kappa^{(2)}+\mu^{(2)})}(2.74p^4-1.95p^3)\right]^2, \quad (5.15b)$$

$$R_{C,D}=\frac{1.11(\mu^{(1)'}_{C,D})^2 s^2_{C,D}}{(\mu^{(2)})^2[(\delta\kappa/\delta\mu)(2\mu^{(1)'}_{C,D}/\kappa^{(1)'}_{C,D})^2+2]}p^4, \quad (5.15c)$$

$$A = Q_{+B2,+B2} \quad \text{[see (5.8)]}. \quad (5.15d)$$

The other shear modulus $M^{(e)}$ is given by the same expression, except that $Q_{+B2,+B2}$ must be replaced by $Q_{-B2,-B2}$.

## 6. DISCUSSION

We have presented a completely new approach to the calculation of effective elastic constants of composites whose microgeometry is known precisely. In the applications discussed in this article, we were able by rather simple analytical perturbative methods, to obtain an expansion for these constants in powers of $p$ to a rather high order. In particular, we obtained Clausius–Mossotti type formulas for a square lattice of fibers that differ from those that are applicable to a hexagonal lattice (or a random isotropic configuration). We also obtained higher order corrections to those, and were able to discuss the validity of the Clausius–Mossotti approximations.

We would like to stress, however, that we are by no means limited to expanding the elastic constants in powers of $p$. Using the matrix elements of Appendix C, we can take any finite portion of the matrix $Q_{\alpha\beta}$ of (4.11) and find its eigenvalues and eigenvectors numerically. Based on experience with the electrostatic problem (see BERGMAN, 1979b), we are confident that accurate results can be obtained in this way even when the fibers in the array are very nearly touching. Again, based on experience with the electrostatic problem (see KANTOR and BERGMAN, 1982), we are confident that random or quasi-random configurations of cylinders can also be handled effectively.

A different situation occurs when, as it is quite often the case, we do not know the microgeometry of the composite precisely. In that case we cannot hope to calculate $C^{(e)}$ precisely. Nevertheless, if we treat the poles $s_\alpha$ and the weights $F_\alpha$ in (2.25) as free parameters and allow them to vary, we can attempt to find rigorous upper and lower bounds on $F(1)$, and hence on the various effective elastic constants. The representation of (2.25) turns out to be admirably suited for this procedure. A future article will be devoted to the derivation of bounds by this method.

Finally, we would like to note that the elastostatic resonances which play so central a role in our approach are of course, implicit in other discussions of composites. Thus, the resonances of an isolated cylindrical inclusion also appear as singularities of the $t$-

matrix for that system, and the resonances of an array of cylinders also appear as singularities of the $T$-matrix for the array. It is in going from the individual inclusion to the array that we use a procedure that is entirely different from the multiple scattering series of $t$-matrices for the total $T$-matrix, as used, for example, by ZELLER and DEDERICHS (1973).

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## APPENDIX A

In this Appendix we prove that all the eigenvalues $s_\alpha$ and all weights $F_\alpha$ are real, and that the product $F_\alpha \cdot s_\alpha$ is always negative.

Let $|\rho^{(\alpha)}\rangle$ be an eigenstate of (2.18) with the eigenvalue $s_\alpha$. From (2.1), (2.7) and the definition of the resonant state it follows that the strain tensor $\varepsilon^{(\alpha)}$, which corresponds to this state, satisfies

$$\partial_j\left[\left(C^{(2)}_{ijkl}+\frac{1}{s_\alpha}\theta\delta C_{ijkl}\right)\varepsilon^{(\alpha)}_{kl}\right]=0, \tag{A.1}$$

and that the corresponding displacement vector $\mathbf{u}$ vanishes at the surface of the sample. We now form the following integral

$$\int u_i^{(\alpha)*}\,\partial_j\left[\left(C^{(2)}_{ijkl}+\frac{1}{s_\alpha}\theta\delta C_{ijkl}\right)\varepsilon^{(\alpha)}_{kl}\right]\mathrm{d}V=0, \tag{A.2}$$

and add to it a similar expression but with the subscripts $i$ and $j$ interchanged. Integrating by parts, we transfer the $\partial_j$ operator to $u_i^{(\alpha)*}$, the surface integral vanishes, and we are left with

$$\int \varepsilon^{(\alpha)*}\left(\boldsymbol{C}^{(2)}+\frac{1}{s_\alpha}\theta\delta\boldsymbol{C}\right)\varepsilon^{(\alpha)}\,\mathrm{d}V=0. \tag{A.3}$$

Since $\boldsymbol{C}^{(2)}$ and $\delta\boldsymbol{C}$ are both real symmetric matrices, the eigenvalue must be real even in the case when $\delta\boldsymbol{C}$ is not a positive or negative definite form, i.e., even when $\hat{H}$ is not a hermitian operator.

Since $\varepsilon^{(\alpha)}$ is an eigenstate of a real integral operator [see (2.11)], and $s_\alpha$ is a real eigenvalue, the real and imaginary parts of $\varepsilon^{(\alpha)}$ are also eigenstates with the same eigenvalue. By a Gram–Schmidt-type orthogonalization process we can construct a complete bi-orthogonal set in which the right eigenstates have the form $\mathrm{A}_\alpha\boldsymbol{K}\varepsilon^{(\alpha)}$, where $\varepsilon^{(\alpha)}$ is a *real* tensor and $\mathrm{A}_\alpha$ is a normalization constant, and the left eigenstates have the form $\mathrm{A}_\alpha^*\boldsymbol{K}^*\varepsilon^{(\alpha)}$ (in the case of a non-degenerate eigenvalue this procedure is unnecessary). The normalization condition is

$$1=\mathrm{A}_\alpha^2\int\theta\varepsilon^{(\alpha)*}\boldsymbol{K}^2\varepsilon^{(\alpha)}\,\mathrm{d}V=\mathrm{A}_\alpha^2\int\theta\varepsilon^{(\alpha)}\delta\boldsymbol{C}\varepsilon^{(\alpha)}\,\mathrm{d}V. \tag{A.4}$$

From this it follows that $\mathrm{A}_\alpha$ is a pure real or pure imaginary number, depending upon the sign of the integral $\int\theta\varepsilon^{(\alpha)}\delta\boldsymbol{C}\varepsilon^{(\alpha)}\,\mathrm{d}V$. Comparing (A.3) with (A.4) we find that, since $\boldsymbol{C}^{(2)}$ is a positive definite matrix,

$$\operatorname{sgn}\mathrm{A}_\alpha^2=\operatorname{sgn}\int\theta\varepsilon^{(\alpha)}\delta\boldsymbol{C}\varepsilon^{(\alpha)}\,\mathrm{d}V=-\operatorname{sgn}s_\alpha. \tag{A.5}$$

From (2.26) we find

$$F_\alpha=\frac{1}{V}\mathrm{A}_\alpha\int\varepsilon^0\delta\boldsymbol{C}\varepsilon^{(\alpha)}\,\mathrm{d}V\cdot\mathrm{A}_\alpha\int\varepsilon^{(\alpha)}\delta\boldsymbol{C}\varepsilon^0\,\mathrm{d}V=\frac{\mathrm{A}_\alpha^2}{V}\left(\int\varepsilon^0\delta\boldsymbol{C}\varepsilon^{(\alpha)}\,\mathrm{d}V\right)^2 \tag{A.6}$$

and hence that $F_\alpha$ is real and that

$$\operatorname{sgn}F_\alpha=-\operatorname{sgn}s_\alpha. \tag{A.7}$$

In the case of degenerate eigenvalues $s_\alpha$, these statements are only guaranteed to hold for the total weight $F_\alpha$ of the resonance at $s_\alpha$.

Since $\boldsymbol{C}^{(1)}$ and $\boldsymbol{C}^{(2)}$ are positive definite tensors, we can easily find from (A.3) that $s_\alpha$ cannot exceed 1. If $\delta\boldsymbol{C}$ is a positive (negative) definite tensor, then $s_\alpha$ is negative (positive).

## APPENDIX B

In this Appendix we describe the main steps in the calculation of the eigenstates of an infinitely long circular cylinder embedded in an infinite host medium. Both the cylinder and host materials are assumed to be isotropic.

Since this 2D problem is invariant under rotations about the cylinder axis, this causes some of the eigenvalues of (2.18) to be infinitely degenerate. In constructing a complete set of bi-orthogonal eigenstates of $\hat{H}$, it is convenient to choose them to be eigenstates of the infinitesimal rotation operator $\hat{J}$ as well. The form in which $\hat{J}$ operates on a strain tensor is given by

$$\hat{J}\varepsilon \equiv \left[ \begin{pmatrix} 0 & 0 & -2 \\ 0 & 0 & 2 \\ 1 & -1 & 0 \end{pmatrix} - i\frac{\partial}{\partial\phi} \right] \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{12} \end{pmatrix} \tag{B.1}$$

where $\phi$ is the azimuthal angle in the plane. It can easily be verified that $\hat{J}$ is hermitian under the scalar product defined by (2.17) and that $\hat{H}$ and $\hat{J}$ commute.

In order to solve for the eigenstates, we use the methods commonly used in 2D elastostatic problems (see, e.g. SOKOLNIKOFF, 1956, pp. 257–282), which are slightly modified, because, at this stage, we allow the eigenstates to be complex. The most general solution of a 2D elastostatic problem in an isotropic medium may be expressed in the form

$$u_1(x_1, x_2) = \frac{1}{2\mu}(\chi\phi - z^*\phi' - \psi + \chi\Delta^* - z\Delta'^* - \gamma),$$

$$u_2(x_1, x_2) = \frac{i}{2\mu}(-\chi\phi - z^*\phi' - \psi + \chi\Delta^* + z\Delta'^* + \gamma), \tag{B.2}$$

where $u_1$, and $u_2$ are the components of the 2D displacement vector, the elastostatic potentials $\phi$, $\psi$, $\Delta$ and $\gamma$ are analytic functions of the complex variable $z = x_1 + ix_2$, a prime denotes differentiation and $\chi = 1 + 2\mu/\kappa$.

The eigenvalues of $\hat{J}$ are all the integers $m = 0, \pm 1, \pm 2, \ldots$ and the elastostatic potentials corresponding to its $m \geqslant 0$ eigenstates are

$$\begin{aligned}
&\phi^{(m)} = A_1 z^{m+1}, \quad \psi^{(m)} = A_2 z^{m-1}, \quad \Delta^{(m)} = A_3/z^{m-1}, \quad \gamma^{(m)} A_4/z^{m+1}, \quad \text{for } m \geqslant 2 \\
&\phi^{(1)} = A_5 z^2, \quad \psi^{(1)} = A_6 \ln z + A_7, \quad \Delta^{(1)} = A_3 \ln z + A_9, \quad \gamma^{(1)} = A_{10}/z^2, \quad \text{for } m = 1 \\
&\phi^{(0)} = A_{11} z, \quad \psi^{(0)} = A_{12}/z, \quad \Delta^{(0)} = A_{13} z, \quad \gamma^{(0)} = A_{14}/z, \quad \text{for } m = 0.
\end{aligned} \tag{B.3}$$

For $m = -|m|$ eigenstates we must replace $\mathbf{u}^{(m)}$ as produced by the above potentials by its complex conjugate. The coefficients $A_i$ are arbitrary if we only require these functions to be eigenstates of $\hat{J}$. Their values are however determined when we require that these functions also be eigenstates of $\hat{H}$, that they decrease to zero for $|z| \to \infty$, and that they be non-singular everywhere else. This determines certain linear combinations of these functions inside and outside the cylinder. From the continuity conditions at the cylinder surface we finally get four homogeneous equations with four unknowns for every value of $m$. Setting the determinant equal to zero leads to the resonance values of $\kappa^{(1)\prime}$, $\mu^{(1)\prime}$ in terms of $\kappa^{(2)}$, $\mu^{(2)}$.

For $|m| \geqslant 2$ the resonance values satisfy either (3.7) or (3.10), for $|m| = 1$ they satisfy (3.10), and for $m = 0$ they satisfy (3.4). The four curves in $\kappa, \mu$ space are shown in Fig. 1. For a problem with given values of $\kappa^{(1)}, \kappa^{(2)}, \mu^{(1)}, \mu^{(2)}$ the values taken by $\kappa^{(1)\prime}$ and $\mu^{(1)\prime}$ must also lie on the straight lines given by

$$\begin{aligned}
\kappa^{(1)\prime} &= \kappa^{(2)} + \frac{1}{s}\delta\kappa, \\
\mu^{(1)\prime} &= \mu^{(2)} + \frac{1}{s}\delta\mu.
\end{aligned} \tag{B.4}$$

Consequently, the actual resonance values of $\kappa^{(1)\prime}$ and $\mu^{(1)\prime}$ in a given problem are the intersection points of that straight line with the four curves of Fig. 1. Thus there are at most four different eigenvalues, denoted by $s_A, s_B, s_C, s_D$ [(3.5), (3.8), (3.11)] in correspondence with the curves of Fig. 1. Correspondingly, there are four pairs of resonance elastic constants $\kappa_A^{(1)\prime}, \mu_A^{(1)\prime}; \kappa_B^{(1)\prime}, \mu_B^{(1)\prime}$; etc.

Instead of using complex $\varepsilon$'s we shall use the linear combinations $(\varepsilon^{(m)}+\varepsilon^{(-m)})$ and $-(\varepsilon^{(m)}-\varepsilon^{(-m)})$, i.e. the real and imaginary parts of $\varepsilon^{(m)}$, for B-, C- and D-type states (in the A-type state there is no degeneracy, and therefore $\varepsilon$ is automatically real). These states are no longer eigenstates of $\hat{J}$, but they are still eigenstates of $\hat{J}^2$, and at the same time eigenstates of the reflection operator through the $x_1$-axis. The real and imaginary parts of $\varepsilon^{(m)}$ have eigenvalues $+1$ and $-1$ respectively, for this operator. Multiplying the resonance strain tensors by $\boldsymbol{K}$ [see (2.12) and (2.13)], which in this case is given by

$$\boldsymbol{K}_{ijkl} = \frac{1}{\sqrt{2}}[\sqrt{(\delta\kappa)}-\sqrt{(\delta\mu)}]\delta_{ij}\delta_{kl}+\sqrt{(2\delta\mu)}\boldsymbol{I}_{ijkl}, \tag{B.5}$$

we obtain the eigenstates $\rho^{(\alpha)}$, which are given by (3.6), (3.9) and (3.12). In Appendix A we explained how to construct the set of left eigenstates and how they should be normalized.

## APPENDIX C

In this Appendix we list expressions for the overlap integrals between a left eigenstate of one cylinder situated at the origin and a right eigenstate of another cylinder located at the point $z$ in the complex plane. The coefficients A, which occur in the formulas were defined in (3.9b) and (3.12b). The step function $\theta_0$ corresponds to the cylinder at the origin; $R$ is the radius of the cylinders; $\binom{m}{n}$ is a binomial coefficient; $\mu_{C,D}^{(1)\prime}$ and $\kappa_{C,D}^{(1)\prime}$ are resonance values of $\mu^{(1)\prime}$ and $\kappa^{(1)\prime}$, as defined in Appendix B; and the notation $|\rho^{(\pm C,Dm)}\rangle$ means that we can take any possible combination of superscripts, e.g. $|\rho^{(+Cm)}\rangle$, $|\rho^{(-Dm)}\rangle$ etc. The matrix element defined by (4.6) is symmetric, and can be calculated with the help of an overlap integral in two different ways

$$\begin{aligned}\langle\tilde{\rho}^{b(\beta)}|\theta_b\hat{H}\theta_a|\rho^{a(\alpha)}\rangle &= s_{a\alpha}\langle\tilde{\rho}^{b(\beta)}|\theta_b|\rho^{a(\alpha)}\rangle \\ &= s_{b\beta}\langle\tilde{\rho}^{b(\beta)}|\theta_a|\rho^{a(\alpha)}\rangle.\end{aligned} \tag{C.1}$$

Therefore the overlap integrals which are not listed below may be obtained by using (C.1).

$$\langle\tilde{\rho}^{(A0)}|\theta_0|\rho^{(A0)}\rangle = 0, \tag{C.2}$$

$$\begin{aligned}\langle\tilde{\rho}^{(+Bm)}|\theta_0|\rho^{(+Bn)}\rangle &= -\langle\tilde{\rho}^{(-Bm)}|\theta_0|\rho^{(-Bn)}\rangle \\ &= A_{Bm}A_{Bn}\frac{2\pi R^{2(m+n-2)}}{1+2\mu^{(2)}/\kappa^{(2)}}(-1)^n\,\mathrm{Re}\left[\binom{m+n}{n}\frac{R^2}{z^{m+n}}-\binom{m+n-2}{m-1}\frac{|z|^2}{z^{m+n}}\right],\end{aligned} \tag{C.3}$$

$$\begin{aligned}\langle\tilde{\rho}^{(-Bm)}|\theta_0|\rho^{(+Bn)}\rangle &= -\langle\tilde{\rho}^{(+Bm)}|\theta_0|\rho^{(-Bn)}\rangle \\ &= A_{Bm}A_{Bn}\frac{2\pi R^{2(m+n-2)}}{1+2\mu^{(2)}/\kappa^{(2)}}(-1)^n\,\mathrm{Im}\left[\binom{m+n}{n}\frac{R^2}{z^{m+n}}-\binom{m+n-2}{m-1}\frac{|z|^2}{z^{m+n}}\right],\end{aligned} \tag{C.4}$$

$$\langle\tilde{\rho}^{(\pm C,Dm)}|\theta_0|\rho^{(\pm C,Dn)}\rangle = 0, \tag{C.5}$$

$$\langle\tilde{\rho}^{(A0)}|\theta_0|\rho^{(\pm C,Dm)}\rangle = 0, \tag{C.6}$$

$$\langle\tilde{\rho}^{(A0)}|\theta_0|\rho^{(\pm Bm)}\rangle = A_{Bm}\frac{\sqrt{(2\pi)}R^{2m-1}}{1+\kappa^{(2)}/2\mu^{(2)}}\left(\frac{\delta\kappa}{\delta\mu}\right)^{1/2}(-1)^m\begin{Bmatrix}\mathrm{Re}\\ \mathrm{Im}\end{Bmatrix}\frac{1}{z^{*m}}, \tag{C.7}$$

$$\langle \tilde{\rho}^{(+\mathrm{Bm})} | \theta_0 | \rho^{(\mathrm{A0})} \rangle = \mathrm{A}_{\mathrm{Bm}} \sqrt{(2\pi)} R^{2m-1} \left( \frac{\delta\mu}{\delta\kappa} \right)^{1/2} \mathrm{Re} \frac{1}{z^m}, \tag{C.8}$$

$$\begin{aligned} \langle \tilde{\rho}^{(+\mathrm{Bm})} | \theta_0 | \rho^{(+\mathrm{C,Dn})} \rangle &= -\langle \tilde{\rho}^{(-\mathrm{Bm})} | \theta_0 | \rho^{(-\mathrm{C,Dn})} \rangle \\ &= \mathrm{A}_{\mathrm{Bm}} \mathrm{A}_{\mathrm{C,Dn}} \frac{2\pi R^{2(m+n)} \mu_{\mathrm{C,D}}^{(1)\prime}}{(m-1)\mu^{(2)}} (-1)^{n+1} \binom{n+m-1}{m-2} \mathrm{Re} \frac{1}{z^{m+n}}, \end{aligned} \tag{C.9}$$

$$\begin{aligned} \langle \tilde{\rho}^{(-\mathrm{Bm})} | \theta_0 | \rho^{(+\mathrm{C,Dn})} \rangle &= -\langle \tilde{\rho}^{(+\mathrm{Bm})} | \theta_0 | \rho^{(-\mathrm{C,Dn})} \rangle \\ &= \mathrm{A}_{\mathrm{Bm}} \mathrm{A}_{\mathrm{C,Dn}} \frac{2\pi R^{2(m+n)} \mu_{\mathrm{C,D}}^{(1)\prime}}{(m-1)\mu^{(2)}} (-1)^{n+1} \binom{n+m-1}{m-2} \mathrm{Im} \frac{1}{z^{m+n}}. \end{aligned} \tag{C.10}$$

## Appendix D

In this Appendix we discuss the calculation of lattice sums of dipole–dipole interactions. We take an approach that is analogous to the one often used in electrostatics for calculating the sum over dipole–dipole interactions, which leads to the so-called "Lorentz local field" (see, e.g. Ashcroft and Mermin, 1976).

The important properties of the elastic dipole states of an isolated cylinder are that $\varepsilon^{(\alpha)}$ is constant inside the cylinder, and that the eigenvalue $s_{a\alpha}$ is independent of the cylinder radius. If we define the elastic polarization density of the cylinder by

$$P_{ij}^{a(\alpha)} \equiv \frac{1}{s_{a\alpha}} \theta_a \delta C_{ijkl} \varepsilon_{kl}^{a(\alpha)} \tag{D.1}$$

then we can find $\varepsilon$ everywhere else by solving the equation

$$\partial_j C_{ijkl}^{(2)} \varepsilon_{kl}^{a(\alpha)} = -\partial_j P_{ij}^{a(\alpha)} \tag{D.2}$$

which is simply (2.1) and (2.7) rewritten in a different way. The sum of dipole–dipole interactions between all the other cylinders and the one at the origin can be written in terms of an overlap integral over the volume of that cylinder, in which the integral is the product of $\rho$ of that cylinder and the $\rho$ due to all other cylinder-dipoles. The latter quantity, denoted by $\rho^{\mathrm{loc}} = \boldsymbol{K}\varepsilon^{\mathrm{loc}}$, is calculated by considering separately the contribution of the nearby cylinders, i.e., those that lie within a circle of radius $L$ around the origin ($L$ must be much larger than the cylinder radii and the intergrain separations), and that of the distant cylinders:

$$\varepsilon^{\mathrm{loc}} = \varepsilon_{\mathrm{near}}^{\mathrm{loc}} + \varepsilon_{\mathrm{far}}^{\mathrm{loc}}. \tag{D.3}$$

In order to calculate the far contribution, we may replace the actual inhomogeneous polarization density for $r > L$ in (D.2) by its volume average. That would lead to a solution for $\varepsilon$ denoted by $\varepsilon_{\mathrm{far}}^{\mathrm{macro}}$. If we made the same replacement for $r < L$ in (D.2), we would obtain the solution denoted by $\varepsilon_{\mathrm{near}}^{\mathrm{macro}}$. Finally, if we replace the inhomogeneous $P_{ij}$ everywhere by its (homogeneous) volume average, the solution of (D.2) would simply be $\varepsilon \equiv 0$ (due to the zero boundary conditions). Therefore the sum $\varepsilon_{\mathrm{near}}^{\mathrm{macro}} + \varepsilon_{\mathrm{far}}^{\mathrm{macro}}$ must vanish, and we can conclude that

$$\varepsilon_{\mathrm{far}}^{\mathrm{loc}} = \varepsilon_{\mathrm{far}}^{\mathrm{macro}} = -\varepsilon_{\mathrm{near}}^{\mathrm{macro}} \tag{D.4}$$

and hence

$$\varepsilon^{\mathrm{loc}} = \varepsilon_{\mathrm{near}}^{\mathrm{loc}} - \varepsilon_{\mathrm{near}}^{\mathrm{macro}}. \tag{D.5}$$

In order to evaluate $\varepsilon_{\mathrm{near}}^{\mathrm{macro}}$ close to the origin, we note that this is again a strain field in a kind of cylinder inclusion at the origin (a very large one—its radius is $L$!) that is entirely due to the uniform polarization density $\frac{1}{s_{a\alpha}} p\, \delta C \varepsilon^{a(\alpha)}$ inside that cylinder. This is reminiscent of the situation

we described earlier for the actual cylindrical inclusion at the origin $a$, where the strain field could be viewed as resulting from a uniform polarization density $\frac{1}{S_{a\alpha}}\delta C\varepsilon^{a(\alpha)}$ inside the cylinder. Consequently, we may conclude that $\varepsilon^{\text{macro}}_{\text{near}}$ is the same as $\varepsilon^{a(\alpha)}$, except for the factor $p$, namely

$$\varepsilon^{\text{macro}}_{\text{near}} = p\varepsilon^{a(\alpha)} \tag{D.6}$$

at all points that are inside both cylinders (the large one and the small one).

When this result is used to substitute for the sum of contributions to $\varepsilon$ from all the dipoles except the one at the origin, we find

$$\begin{aligned} Q_{\beta\alpha} &= \sum_{\substack{a \\ 0 \neq |\mathbf{a}-\mathbf{b}|}} \langle \tilde{\rho}^{b(\beta)} | \theta_b \hat{H} \theta_a | \rho^{a(\alpha)} \rangle \\ &= \sum_{\substack{a \\ 0 \neq |\mathbf{a}-\mathbf{b}| < L}} \langle \tilde{\rho}^{b(\beta)} | \theta_b \hat{H} \theta_a | \rho^{a(\alpha)} \rangle - p \langle \rho^{b(\beta)} | \theta_b \hat{H} \theta_b | \rho^{a(\alpha)} \rangle \\ &= \sum_{\substack{a \\ 0 \neq |\mathbf{a}-\mathbf{b}| < L}} \langle \tilde{\rho}^{b(\beta)} | \theta_b \hat{H} \theta_a | \rho^{a(\alpha)} \rangle - a_{a\alpha} p \delta_{\alpha\beta}. \end{aligned} \tag{D.7}$$

In this equation, $L$ must be large enough so that the use of an average polarization density for $r > L$ is a good approximation. In practice, one sums the series over a set of circles with larger and larger $L$ until convergence is obtained [see (5.1)].