

New extremal inclusions and their applications to two-phase composites

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Abstract

In this paper, we find a class of special inclusions that have the same property with respect to second order linear partial differential equations as holds for ellipsoids. That is, in the simplest case and in physical terms, constant magnetization of the inclusion implies constant magnetic field on the inclusion. The special inclusions are found as solutions of a simple variational inequality. This variational inequality allows us to prescribe the connectivity and periodicity properties of the inclusions. For example we find periodic arrays of inclusions in two and three dimensions for which constant magnetization of the inclusions implies constant magnetic field on the inclusions. The volume fraction of the inclusions can be any number between zero and one. We find such inclusions with any finite number of components and components that are multiply connected. These special inclusions enjoy many useful properties with respect to homogenization and energy minimization. For example, we use them to give new results on a) the effective properties of two-phase composites and b) optimal bounds and optimal structures for two-phase composites.

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1. Introduction

POISSON [47] found a remarkable property of ellipsoids: given a uniformly magnetized ellipsoid, the induced magnetic field is uniform inside the ellipsoid. Explicit expressions for this field were obtained by MAXWELL [41]. ESHELBY [13, 12] exploited a similar result in the linear theory of elasticity. Eshelby's solution asserts that a uniform eigenstrain on an ellipsoidal subregion in an infinite elastic medium induces uniform stress inside the ellipsoid (see also, MURA [45]). In this paper we find other shapes besides ellipsoids with these properties.

The relevant problem can be formulated as the following partial differential equation for $\mathbf{v} : \mathbb{R}^n \rightarrow \mathbb{R}^m$:

$$\operatorname{div}[\mathbf{L}\nabla\mathbf{v} + \mathbf{P}\chi_\Omega] = 0 \quad \text{on } \mathbb{R}^n, \quad (1-1)$$

where $\mathbf{P} \in \mathbb{R}^{m \times n}$, and the tensor $\mathbf{L} : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}^{m \times n}$ is assumed to be self-adjoint and positive-definite. Also, $\Omega \subset \mathbb{R}^n$ is called the inclusion and χ_Ω is the characteristic function of Ω . In the application to ferromagnetism, $m = 1$, $\nabla\mathbf{v}$ is the magnetic field, \mathbf{P} is the magnetization, and \mathbf{L} is the identity. In applications to electrostatics, $m = 1$, $\nabla\mathbf{v}$ is the electric field, \mathbf{P} is the polarization, and \mathbf{L} is the inverse of the product of the permittivity of free space and the susceptibility tensor. In the application to linearized elasticity, $m = n$, $\nabla\mathbf{v}$ is the displacement gradient, \mathbf{P} is the eigenstress and \mathbf{L} is the elasticity tensor.

In the theory of composites and in fracture mechanics a related problem, called the *inhomogeneous* Eshelby inclusion problem, appears often. The governing equations for this problem are

$$\operatorname{div}[\mathbf{L}(\mathbf{x}, \Omega)(\nabla\mathbf{v}(\mathbf{x}) + \mathbf{F}\chi_\Omega)] = 0 \quad \text{on } \mathbb{R}^n, \quad (1-2)$$

where $\mathbf{F} \in \mathbb{R}^{m \times n}$ is the eigenstrain and the elasticity tensor

$$\mathbf{L}(\mathbf{x}, \Omega) = \begin{cases} \mathbf{L}_1 & \mathbf{x} \in \Omega, \\ \mathbf{L}_2 & \mathbf{x} \in \mathbb{R}^n \setminus \Omega. \end{cases} \quad (1-3)$$

The inhomogeneous Eshelby inclusion problem concerns two different elastic materials, one inside the inclusion, and an imposed eigenstrain \mathbf{F} on the inclusion. ESHELBY [13] realized that under suitable mild hypotheses on the elasticity tensors the homogeneous problem (1-1) can be used to solve inhomogeneous problem (1-2) provided that the induced field $\nabla\mathbf{v}$ for the homogeneous problem (1-1) is constant on Ω . It is this relation between

(1-2) and (1-1) that allows us to use the special inclusions to obtain optimal bounds for composites.

The requirement that a solution \mathbf{v} of problem (1-1) satisfy $\nabla \mathbf{v} = \text{constant}$ on Ω places strong restrictions on the region Ω . The main purpose of this paper is to find special regions with this property in the periodic and other cases, including cases in which Ω is multiply connected.

Since $\nabla \mathbf{v}$ being constant on Ω leads to great simplification, ellipsoids play a central role in the theory of composites (CHRISTENSEN [8]; MILTON [43]), in micromechanics (MURA [45]) and in experimental measurements (BROWN [6]). The uniformity of the induced field can also be used to simplify free energy minimization problems that arise in theories of ferroelectric and magnetostrictive materials (DESIMONE & JAMES [10]; BHATTACHARYA & LI [4]; LIU, JAMES & LEO [37]), and this was our original motivation for developing the theory of E-inclusions. Roughly speaking, even though these are non-convex variational problems, the special properties of ellipsoids are used to show that certain weak limits of minimizing sequences are uniform, and this allows one to find, and also to minimize, the relaxed energy. Two or more ellipsoids do not enjoy this special property. Thus in many of these applications, only one ellipsoid can be present in the model, and therefore the results apply either to isolated ellipsoids or to composites in the dilute limit. In most if not all of these cases it is not an ellipsoid *per se* that is being used but only its property of having uniform field, when it is uniformly magnetized. Many authors have speculated on the possibility that other regions may have this property (MURA [46]), and that, if so, their analysis would also apply to those regions.

We now define an **E-inclusion**, which is the mathematically natural generalization of an ellipsoid in this context¹ (see LIU, JAMES & LEO [38]). We note that, while these definitions concern the scalar-valued case, we will show (Section 4) that they apply to many vector-valued examples of the type described above. Separate but closely related definitions of E-inclusions are given for the periodic and nonperiodic cases. More general situations are discussed in Section 5.

Definition 1. Let measurable Ω_i with $|\partial\Omega_i| = 0$ ($i = 1, \dots, N$) be bounded and mutually disjoint subsets of \mathbb{R}^n , and let $\mathbb{K} = (\mathbf{Q}_1, \dots, \mathbf{Q}_N)$ be an array of N symmetric $n \times n$ matrices.

- i) $(\Omega_1, \dots, \Omega_N)$ is an **E-inclusion** corresponding to \mathbb{K} if there is a solution $u \in W_{loc}^{2,2}(\mathbb{R}^n)$ of problem

$$\Delta u = \sum_{i=1}^N p_i \chi_{\Omega_i} \quad \text{on } \mathbb{R}^n, \quad p_i = \text{Tr}(\mathbf{Q}_i), \quad (1-4)$$

¹ The terminology ‘‘E-inclusions’’ refers to three associations: 1) this study was motivated by the Eshelby inclusion problem as described above; 2) they are a generalization of ellipsoids, and, conversely, ellipsoids can be regarded as the dilute limits of special periodic E-inclusions; 3) they are extremal structures for a broad class of energy minimization problems for multiphase composites.

satisfying

$$\nabla \nabla u = \mathbf{Q}_i \quad \text{on } \Omega_i \setminus \partial \Omega_i \quad \forall i = 1, \dots, N. \quad (1-5)$$

The interpretation of the Poisson equation (1-4) is in terms of the Newtonian potential representation for u , see (4.1) of GILBARG & TRUDINGER [17].

- ii) Let a Bravais lattice $\mathcal{L} = \{\sum_{i=1}^n \nu_i \mathbf{e}_i : \nu_i \in \mathbb{Z} \text{ and } \mathbf{e}_1, \dots, \mathbf{e}_n \in \mathbb{R}^n \text{ are linearly independent}\}$ with an open unit cell $Y = \{\sum_{i=1}^n x_i \mathbf{e}_i : 0 < x_i < 1\}$ be given. Assume $\Omega = \cup_{i=1}^N \Omega_i \subset Y$. Then the set $\Omega_{per} = \cup_{\mathbf{r} \in \mathcal{L}} \{\mathbf{r} + \Omega\}$ is a **periodic E-inclusion** corresponding to \mathbb{K} if there is a solution $u \in W_{per}^{2,2}(Y)$ of

$$\begin{cases} \Delta u = \sum_{i=0}^N p_i \chi_{\Omega_i} & \text{on } Y, \quad p_i = \text{Tr}(\mathbf{Q}_i), \\ \text{periodic boundary conditions} & \text{on } \partial Y \end{cases} \quad (1-6)$$

satisfying

$$\nabla \nabla u = \mathbf{Q}_i \quad \text{on } \Omega_i \setminus \partial \Omega_i \quad \forall i = 1, \dots, N, \quad (1-7)$$

where $\Omega_0 = Y \setminus \Omega$, and $p_0 \in \mathbb{R}$ is chosen such that $\sum_{i=0}^N p_i \theta_i = 0$. Here $\theta_i = |\Omega_i|/|Y|$ is the volume fraction of Ω_i in Y .

It is desirable to allow the arbitrary set of measure zero on the boundaries in the definition of E-inclusions, because of examples like Fig. 5. The $W^{2,2}$ regularity in these definitions is standard for these equations. In fact, using L^p estimates for the Laplace operator we see that $u \in W_{loc}^{2,p}$ (resp., $W_{per}^{2,p}$) for any $1 < p < \infty$ since the right-hand side of (1-4) (resp., (1-6)) is bounded in L^∞ (GILBARG & TRUDINGER [17], page 235).

Equations (1-1) and (1-2) and their periodic counterparts are closely related to equations (1-4) and (1-6), respectively. In particular, in the magnetic case (recall $m = 1$), $\mathbf{v} = \mathbf{P} \cdot \nabla u$, and the magnetization on inclusion Ω_i ($i = 1, \dots, N$) is $(p_i - p_0)\mathbf{P}$ and zero elsewhere. Also, each matrix in $(\mathbf{Q}_1, \dots, \mathbf{Q}_N)$ plays the same role as the conventional *demagnetization matrix* does for an isolated ellipsoid. The demagnetization matrix defines the linear transformation that maps the magnetization \mathbf{P} to the magnetic field $\nabla \mathbf{v}$ when Ω is an ellipsoid. Further discussion of the relation between (1-1), (1-2) and (1-4), (1-6) is given in Section 4.1.

Besides ellipsoids, examples of E-inclusions include the well-known construction of VIGDERGAUZ [52] for two dimensional periodic E-inclusions which are simply connected in one unit cell. Other examples of which we are aware include two dimensional two-component E-inclusions in a forthcoming paper of KANG & MILTON [27]. While considering the effective properties of an elastic plate with a periodic array of “equal-strength” holes, Vigdergauz found his construction using complex variable methods. MILTON ([43], page 481) subsequently reduced the construction of Vigdergauz to a Dirichlet problem. GRABOVSKY & KOHN [20] gave a concise derivation of the Vigdergauz construction and showed that it is an optimal structure for

two-phase composites. These results on the status of E-inclusions as optimal structures in homogenization theory, and the results mentioned above on energy minimization, show that E-inclusions have a more fundamental relation to the underlying equations than merely as a method of simplification. We present several applications of this type in Section 4.

In Section 2 we present a general method for constructing E-inclusions. They are found as solutions of a simple variational inequality with a piecewise quadratic obstacle. The region where the minimizer touches the obstacle defines the E-inclusion. The existence and regularity of minimizers for this variational inequality are adapted from the textbook of FRIEDMAN [15]. We further show that periodic E-inclusions corresponding to a single negative-semidefinite matrix ($N = 1$) can be constructed in all dimensions and with any volume fraction. The lattice vectors defining the periodicity can be arbitrarily prescribed. In two dimensions, one family of these periodic E-inclusions specialize to the Vigdergauz microstructure. By varying the piecewise quadratic obstacle in the variational inequality, a variety of more general E-inclusions can be produced. For example, we can construct periodic E-inclusions with multiply connected components. In Section 3 we present a numerical scheme for calculating periodic E-inclusions and various examples of the calculated periodic E-inclusions. In Section 4.1 we solve the periodic Eshelby inclusion problem and explicitly calculate the effective properties of two-phase composites with periodic E-inclusion structures. In Section 4.2 explicit bounds for the effective properties of two-phase composites are derived and are shown to be attained by the periodic E-inclusions. In Section 5 we introduce a generalized concept of E-inclusions called sequential E-inclusions in terms of gradient Young measure. We finish with a summary of our results.

2. A method for constructing special inclusions

2.1. Existence of periodic E-inclusions

In this section, we present a method for the construction of E-inclusions. Readers who are more interested in the examples and applications of E-inclusions may skip to Sections 3 and 4.

A general method for constructing special inclusions is based on a *variational inequality* (KINDERLEHRER & STAMPACCHIA [33]; FRIEDMAN [15]). For periodic E-inclusions in \mathbb{R}^n ($n \geq 1$), we consider

$$G_f(u_f) \equiv \min_{u \in K_{per}} \left\{ G_f(u) \equiv \int_Y \left[\frac{1}{2} |\nabla u|^2 + fu \right] d\mathbf{x} \right\}, \quad (2-1)$$

where $f > 0$ is a constant and the admissible set $K_{per} = \{u \in W_{per}^{1,2}(Y) : u(\mathbf{x}) \geq \phi_{per}(\mathbf{x}) \text{ a.e. on } \mathbb{R}^n\}$. This type of minimization problem is also known as a *free-boundary obstacle problem* and the given function ϕ_{per} is

called the *obstacle*. Here and afterwards, Y is an open unit cell associated with a Bravais lattice \mathcal{L} as defined above. We further assume

$$\begin{aligned} \phi_{per} &\in C_{per}^{0,1}(Y) \quad \text{and} \\ \frac{\partial^2 \phi_{per}}{\partial \xi^2} &\geq -C \text{ in the sense of distributions on } \mathbb{R}^n, \end{aligned} \quad (2-2)$$

where ξ is any unit vector in \mathbb{R}^n , $\partial/\partial \xi$ denotes the directional derivative and $C > 0$ is a constant. This means that for any $\varphi \in C_c^\infty(\mathbb{R}^n)$ and any unit vector $\xi \in \mathbb{R}^n$,

$$\int [\phi_{per} + \frac{1}{2}C|\mathbf{x}|^2] \frac{\partial^2 \varphi}{\partial \xi^2} d\mathbf{x} \geq 0,$$

see FRIEDMAN ([15], page 28).

If $v \in K_{per}$, from the convexity of K_{per} we have $w_\varepsilon = u_f + \varepsilon(v - u_f) \in K_{per}$ for all $\varepsilon \in (0, 1)$. Since u_f being a minimizer implies $\frac{1}{\varepsilon}[G_f(w_\varepsilon) - G_f(u_f)] \geq 0$, sending ε to 0 we obtain a necessary condition for a minimizer

$$\int_Y [\nabla u_f \cdot \nabla(v - u_f) + f(v - u_f)] d\mathbf{x} \geq 0 \quad \forall v \in K_{per}. \quad (2-3)$$

The coincident set Ω_{per}^f and noncoincident set N_{per}^f are defined as

$$\Omega_{per}^f := \{\mathbf{x} \in \mathbb{R}^n : u_f(\mathbf{x}) = \phi_{per}(\mathbf{x})\} \quad (2-4)$$

and

$$N_{per}^f := \{\mathbf{x} \in \mathbb{R}^n : u_f(\mathbf{x}) > \phi_{per}(\mathbf{x})\}, \quad (2-5)$$

respectively.

The existence, uniqueness and regularity of the minimizer for the variational inequality (2-1) have been well established, see KINDERLEHRER & STAMPACCHIA [33]; FRIEDMAN [15].

Theorem 1. *The variational inequality (2-1)-(2-2) has a unique minimizer $u_f \in W_{per}^{2,\infty}(Y)$ for all $f > 0$.*

Using this result ($u_f \in W_{per}^{2,\infty}(Y)$), we have that the noncoincident set N_{per}^f is open. For any $\varphi \in C_c^\infty(N_{per}^f) \cup \{\varphi \in C_c^\infty(\mathbb{R}^n) : \varphi \geq 0\}$, there exists small enough $\varepsilon > 0$ such that $v = u_f + \varepsilon\varphi \in K_{per}$. Plugging v into equation (2-3), it then follows that

$$\begin{aligned} -\Delta u_f + f &\geq 0, & u_f &\geq \phi_{per}, & \text{and} \\ (-\Delta u_f + f)(u_f - \phi_{per}) &= 0 & \text{a.e. on } Y. \end{aligned} \quad (2-6)$$

Recalling the definition of periodic E-inclusions in Section 1, we use periodic piecewise quadratic obstacles to construct periodic E-inclusions. First, we assign N quadratic functions q_1, \dots, q_N on Y . Second, we consider

a disjoint measurable subdivision of Y into subsets $\mathcal{U}_1, \dots, \mathcal{U}_N$. We say that $\phi_{per} : \mathbb{R}^n \rightarrow \mathbb{R}$ is a **periodic piecewise quadratic obstacle** if

- (i) ϕ_{per} satisfies (2-2), and
- (ii) $\phi_{per} = q_i$ on \mathcal{U}_i .

In general one may not be able to construct a periodic piecewise quadratic obstacle from given quadratic functions. Below we give two examples of periodic piecewise quadratic obstacles. Both examples use concave quadratic functions. We note that the definition, however, also includes some cases in which some of the q_i are not concave. The latter is important for extending the attainability of the Hashin-Shtrikman bounds for multiphase composites.

Example 1. Let q_1, \dots, q_N be strictly concave quadratic functions defined on \mathbb{R}^n . Then

$$\phi_{per}(\mathbf{x}) = \sup\{q_i(\mathbf{x} + \mathbf{r}) : \mathbf{r} \in \mathcal{L}, i = 1, \dots, N\} \quad (2-7)$$

is a periodic piecewise quadratic obstacle. To see the connection with FRIEDMAN ([15], page 44, Ex.2), consider an open bounded domain D . Using the strict concavity of the q_i , we can write $\phi_{per}|_D$ as the maximum of a finite number of quadratic functions. Then (2-2) is verified on D . Using the arbitrariness of D and the fact that φ in (2-2) has compact support, we see that (2-2) is satisfied on all of \mathbb{R}^n .

Example 2. Assume $N = 1$ and consider a negative semi-definite symmetric matrix $\mathbf{Q}_1 = \mathbf{Q} \neq 0$ and denote by $\mathcal{R}(\mathbf{Q}) \subset \mathbb{R}^n$ the range of \mathbf{Q} . Let $(\mathbf{e}_1, \dots, \mathbf{e}_{n'})$ be a basis of the subspace $\mathcal{R}(\mathbf{Q})$. Then

$$\phi_{per}(\mathbf{x}) = \sup\left\{\frac{1}{2}(\mathbf{x} + \mathbf{r}) \cdot \mathbf{Q}(\mathbf{x} + \mathbf{r}) : \mathbf{r} = \sum_{i=1}^{n'} \nu_i \mathbf{e}_i, \nu_i \in \mathbb{Z}\right\} \quad (2-8)$$

is a periodic piecewise quadratic obstacle. The proof that this construction gives a periodic piecewise quadratic obstacle is similar to that in Example 1.

The definition of the coincident set clearly implies

$$\nabla \nabla u_f(\mathbf{x}) = \nabla \nabla \phi_{per}(\mathbf{x}) \quad \text{on } \Omega_{per}^f \setminus \partial \Omega_{per}^f. \quad (2-9)$$

Further, it has been shown the free boundary $\partial \Omega_{per}^f$ has measure zero in \mathbb{R}^n (FRIEDMAN [15], page 154). From this fact, Theorem 1, and (2-6)-(2-9), it follows that the minimizer $u_f \in W_{per}^{2,\infty}(Y)$ solves the overdetermined problem

$$\begin{cases} \Delta u_f = f \chi_{N_{per}^f} + \Delta \phi_{per} \chi_{\Omega_{per}^f} & \text{a.e. on } Y, \\ \nabla \nabla u_f(\mathbf{x}) = \nabla \nabla \phi_{per}(\mathbf{x}) & \text{on the interior of } \Omega_{per}^f \cap Y, \\ \text{periodic boundary conditions} & \text{on } \partial Y. \end{cases} \quad (2-10)$$

Since ϕ_{per} is a periodic piecewise quadratic obstacle, there exist symmetric matrices $(\mathbf{Q}_1, \dots, \mathbf{Q}_N)$ and mutually disjoint regions $(\Omega_0, \Omega_1, \dots, \Omega_N)$ in Y , which satisfy $|\partial\Omega_i| = 0$ and are well-defined within a set of measure zero, such that

$$\begin{aligned} \Delta u_f &= f & \text{on } \Omega_0 &= Y \setminus (\cup_{i=1}^N \Omega_i) & \text{and} & & (2-11) \\ \nabla \nabla u_f(\mathbf{x}) &= \mathbf{Q}_i & \text{on } \Omega_i &\setminus \partial\Omega_i & \forall i &= 1, \dots, N. \end{aligned}$$

Therefore, we have obtained the following result.

Theorem 2. *Consider the variational inequality (2-1) with a piecewise quadratic obstacle ϕ_{per} . Then the coincident set Ω_{per}^f is a periodic E-inclusion with $p_0 = f$, for any $f > 0$.*

From equation (2-11) and Definition 1, the periodic E-inclusion Ω_{per}^f so constructed corresponds to

$$\mathbb{K} = (\mathbf{Q}_1, \dots, \mathbf{Q}_N) \quad \text{and} \quad \Theta = (\theta_1, \dots, \theta_N),$$

where $\theta_i = |\Omega_i|/|Y|$ is the volume fraction of Ω_i in Y ($i = 0, 1, \dots, N$). Clearly, the volume fractions Θ necessarily satisfy

$$\theta_i \in [0, 1] \text{ for all } i = 1, \dots, N \text{ and } 1 - \theta_0 = \sum_{i=1}^N \theta_i \in (0, 1). \quad (2-12)$$

However, they are not all known *a priori*. Additionally, they satisfy

$$\int_Y \Delta u_f d\mathbf{x} = 0 \implies f\theta_0 + \sum_{i=1}^N p_i \theta_i = 0, \quad (2-13)$$

where $p_i = \text{Tr}(\mathbf{Q}_i)$ ($i = 1, \dots, N$) from the second of (2-11). Since f can be any positive number, equation (2-13) implies that the volume fraction $1 - \theta_0$ of the periodic E-inclusion can be any number between zero and one in the case $N = 1$.

There are non-obvious restrictions on \mathbb{K} and Θ that arise from the definition of a periodic E-inclusion. Let u be the solution of (1-6)-(1-7) appearing in the definition of a periodic E-inclusion. For any $\mathbf{m} \in \mathbb{R}^n$, the divergence theorem implies that

$$\begin{aligned} & \theta_0 \int_{\Omega_0} |(\nabla \nabla u)\mathbf{m}|^2 d\mathbf{x} \\ &= \mathbf{m} \cdot \left[\int_Y \Delta u \nabla \nabla u d\mathbf{x} \right] \mathbf{m} - \sum_{i=1}^N \theta_i \int_{\Omega_i} |(\nabla \nabla u)\mathbf{m}|^2 d\mathbf{x}. \end{aligned} \quad (2-14)$$

We bound the left-hand side of (2-14)

$$\begin{aligned} \theta_0 \int_{\Omega_0} |(\nabla \nabla u) \mathbf{m}|^2 d\mathbf{x} &\geq \theta_0 \mathbf{m} \cdot \left[\int_{\Omega_0} \nabla \nabla u d\mathbf{x} \right]^2 \mathbf{m} \\ &= \frac{1}{\theta_0} \mathbf{m} \cdot \left[\sum_{i=1}^N \theta_i \int_{\Omega_i} \nabla \nabla u d\mathbf{x} \right]^2 \mathbf{m}, \end{aligned}$$

where the equality follows from the periodicity of u

$$\int_Y \nabla \nabla u d\mathbf{x} = 0 \implies \theta_0 \int_{\Omega_0} \nabla \nabla u d\mathbf{x} = - \sum_{i=1}^N \theta_i \int_{\Omega_i} \nabla \nabla u d\mathbf{x}. \quad (2-15)$$

For the first term on the right-hand side of (2-14), since $\Delta u = p_0$ on Ω_0 , we have

$$\begin{aligned} \theta_0 \mathbf{m} \cdot \left[\int_{\Omega_0} \Delta u \nabla \nabla u d\mathbf{x} \right] \mathbf{m} &= p_0 \mathbf{m} \cdot \left[\theta_0 \int_{\Omega_0} \nabla \nabla u d\mathbf{x} \right] \mathbf{m} \\ &= p_0 \mathbf{m} \cdot \left[- \sum_{i=1}^N \theta_i \int_{\Omega_i} \nabla \nabla u d\mathbf{x} \right] \mathbf{m}, \end{aligned}$$

where the second equality is justified by using again (2-15). Therefore, equation (2-14) implies the following restriction on \mathbb{K} and Θ :

$$\sum_{i=1}^N [\theta_0 \text{Tr}(\mathbf{Q}_i) + \sum_{j=1}^N \theta_j \text{Tr}(\mathbf{Q}_j)] \theta_i \mathbf{Q}_i \geq \theta_0 \sum_{i=1}^N \theta_i \mathbf{Q}_i^2 + \left[\sum_{i=1}^N \theta_i \mathbf{Q}_i \right]^2, \quad (2-16)$$

where equations (1-7) and $\theta_0 p_0 = - \sum_{j=1}^N \theta_j \text{Tr}(\mathbf{Q}_j)$ have been used. Also, for two self-adjoint linear mappings, $\mathbf{M}_1 \geq$ (resp., $>$) \mathbf{M}_2 means $\mathbf{M}_1 - \mathbf{M}_2$ is positive semi-definite (resp., positive definite). This convention is followed subsequently. It is not known in general whether \mathbb{K} and Θ satisfying (2-12) and (2-16) can all be achieved by periodic E-inclusions. For many applications, the following question is crucial:

Question 1. *For what values of \mathbb{K} and Θ can we find a periodic E-inclusion?*

For some special cases, the answer to Question 1 is known. The following remark describes such an example.

Remark 1. In the case $N = 1$, equations (2-12) and (2-16) are equivalent to

$$\theta \in (0, 1) \quad \text{and} \quad \mathbf{Q} \geq 0 \text{ or } \mathbf{Q} \leq 0, \quad (2-17)$$

where θ is the volume fraction of a periodic E-inclusion. Note that we have suppressed the subscript “ i ”. Below we verify that a periodic E-inclusion

can be found for any nonzero² \mathbf{Q} and θ satisfying (2-17). If $\mathbf{Q} \leq 0$ but is not equal to the zero matrix, we choose the periodic piecewise quadratic obstacle of Example 2, (2-8). From Theorem 2 and (2-13), it follows that the coincident set Ω_{per}^f is a periodic E-inclusion corresponding to \mathbf{Q} and its volume fraction is $\theta = f/(f - \text{Tr}(\mathbf{Q}))$. Since f can be any positive number, θ can be any number between zero and one.

By replacing u by au ($a \in \mathbb{R}$) in the Definition 1, we see that if Ω_{per} is a periodic E-inclusion corresponding to \mathbf{Q} and θ , then it is also a periodic E-inclusion corresponding to $a\mathbf{Q}$ and θ . The case $\mathbf{Q} \geq 0$ follows from the case $\mathbf{Q} \leq 0$ by setting $a = -1$.

It is often desirable to fix the arbitrary multiplicative constant associated with the matrix $\mathbf{Q} \neq 0$. For future convenience, let us rephrase Remark 1 as the following theorem.

Theorem 3. *Let*

$$\mathbb{Q} := \{X \in \mathbb{R}_{sym}^{n \times n} : X \geq 0 \text{ and } \text{Tr}(X) = 1\}. \quad (2-18)$$

For any matrix $\mathbf{Q} \in \mathbb{Q}$ and any volume fraction $\theta \in (0, 1)$, there exists a periodic E-inclusion Ω_{per} such that the overdetermined problem

$$\begin{cases} \Delta u = \theta - \chi_\Omega & \text{on } Y \\ \nabla \nabla u = -(1 - \theta)\mathbf{Q} & \text{on } \Omega \setminus \partial\Omega \\ \text{periodic boundary conditions} & \text{on } \partial Y \end{cases} \quad (2-19)$$

has a solution in $W_{per}^{2,\infty}(Y)$, where Y is a unit cell, $\Omega = Y \cap \Omega_{per}$ with $|\partial\Omega| = 0$, and $\theta = |\Omega|/|Y|$. Conversely, if the overdetermined problem (2-19) has a solution $u \in W_{per}^{2,\infty}(Y)$ for a nonzero matrix \mathbf{Q} , then the matrix \mathbf{Q} must belong to \mathbb{Q} .

Proof. Only the last statement needs proof, but this follows immediately by taking the trace of the second equation in (2-19), and also by using the inequality (2-16). The space $W_{per}^{2,\infty}$ comes from Theorem 1.

2.2. Existence of nonperiodic E-inclusions for $n \geq 3$

To construct nonperiodic E-inclusions in \mathbb{R}^n , $n \geq 3$, we use the variational inequality

$$G_r(u_r) = \inf_{u \in K_r} \left\{ G_r(u) \equiv \int_{B_r} \frac{1}{2} |\nabla u|^2 dx \right\}, \quad (2-20)$$

where B_r is the open ball centered at the origin of radius r , and the admissible set is

$$K_r = \{v \in W_0^{1,2}(B_r) : v \geq \phi\}. \quad (2-21)$$

² The case $\mathbf{Q} = 0$ is not of interest since it implies $u = \text{const.}$ on \mathbb{R}^n in Definition 1.

We use this variational inequality to find u_r and the coincident set, and then we pass to the limit $r \rightarrow \infty$ to establish the existence of nonperiodic E-inclusions.

Let q_1, \dots, q_N be quadratic functions on \mathbb{R}^n and $\mathcal{U}_1, \dots, \mathcal{U}_N$ a disjoint measurable subdivision of \mathbb{R}^n . As before, we say that $\phi : \mathbb{R}^n \rightarrow \mathbb{R}$ is a **piecewise quadratic obstacle** if

- (i) $\phi \in C^{0,1}(\mathbb{R}^n)$, $\partial^2 \phi / \partial \xi^2 > -C$ on \mathbb{R}^n in distributional sense, for all $|\xi| = 1$,
- (ii) $\phi = q_i$ on \mathcal{U}_i ($i = 1, \dots, N$), and
- (iii) There exists $R_0 > 0$ such that $\phi(\mathbf{x}) < 0$ if $|\mathbf{x}| \geq R_0$.

Here, as above, $\partial / \partial \xi$ denotes the directional derivative. From the established theory (KINDERLEHRER & STAMPACCHIA [33], page 129; FRIEDMAN [15], page 31), we have

Theorem 4. *The variational inequality (2-20) with ϕ being a piecewise quadratic obstacle has a unique minimizer $u_r \in W^{2,\infty}(B_r) \cap W_0^{1,\infty}(B_r)$ for each $r \geq R_0$. Further, the unique minimizer satisfies*

- (i) $\phi \leq u_r \leq \sup\{\phi(\mathbf{x}) : \mathbf{x} \in B_r\}$ on B_r ,
- (ii) The boundary of the coincident set $\Omega_r := \{\mathbf{x} \in B_r : u_r(\mathbf{x}) = \phi(\mathbf{x})\}$ has measure zero in \mathbb{R}^n , and
- (iii) There exists a constant $C > 0$, independent of r , such that

$$\|\nabla \nabla u_r\|_{L^\infty(B_r)} < C. \quad (2-22)$$

By using arguments parallel to those in the derivation of equation (2-6), it can be similarly shown that the minimizer u_r satisfies

$$-\Delta u_r \geq 0, \quad u_r \geq \phi, \quad \text{and} \quad -\Delta u_r(u_r - \phi) = 0 \text{ a.e. on } B_r. \quad (2-23)$$

Thus, the minimizer u_r in fact solves the following overdetermined problem

$$\begin{cases} \Delta u_r = \chi_{\Omega_r} \Delta \phi & \text{a.e. on } B_r, \\ \nabla \nabla u_r = \nabla \nabla \phi & \text{on } \Omega_r \setminus \partial \Omega_r, \\ u_r = 0 & \text{on } \partial B_r. \end{cases} \quad (2-24)$$

A limiting minimizer of problem (2-20) can be defined as follows. Let $r_j \rightarrow +\infty$ be an increasing sequence. From equation (2-22) and $\|u_r\|_{L^\infty(B_R)} < \sup_{B_R} |\phi|$, it follows that for any $r > R > R_0$, there is a constant M , independent of r , such that

$$\|u_r\|_{W^{2,\infty}(B_R)} \leq M. \quad (2-25)$$

Generally, M can depend on R, R_0 and the obstacle ϕ . Since u_{r_j} is uniformly bounded in $W^{2,\infty}(B_R)$ for fixed $R > R_0$, there exists $u_\infty \in W^{2,\infty}(B_R)$ such that, up to a subsequence and without relabeling,

$$u_{r_j} \rightharpoonup u_\infty \text{ weakly}^* \text{ in } W^{2,\infty}(B_R). \quad (2-26)$$

From (2-23) and (2-26), it is easy to verify that

$$-\Delta u_\infty \geq 0, \quad u_\infty \geq \phi, \quad \text{and} \quad -\Delta u_\infty(u_\infty - \phi) = 0 \quad \text{a.e. on } B_R. \quad (2-27)$$

In particular, the first two of (2-27) follow from linearity, while the third of (2-27) is justified by the uniform convergence of $u_r \rightarrow u_\infty$. In fact, we can repeat this argument for a sequence of larger and larger values of R , each time taking further subsequences of u_{r_j} , and thereby obtain a function $u_\infty \in W_{loc}^{2,\infty}(\mathbb{R}^n)$ satisfying (2-26) and (2-27) for any $R > R_0$. Note that equation (2-27) implies that the coincident set $\Omega_\infty := \{\mathbf{x} \in \mathbb{R}^n : u_\infty(\mathbf{x}) = \phi(\mathbf{x})\} \subset B_{R_0}$ have the property that $|\partial\Omega_\infty| = 0$, see FRIEDMAN ([15], page 154).

We claim that u_∞ solves the following overdetermined problem:

$$\begin{cases} \Delta u_\infty = \chi_{\Omega_\infty} \Delta \phi & \text{a.e. on } \mathbb{R}^n, \\ \nabla \nabla u_\infty = \nabla \nabla \phi & \text{on } \Omega_\infty \setminus \partial\Omega_\infty, \\ |u_\infty(\mathbf{x})| \leq \frac{C_0}{|\mathbf{x}|^{n-2}} & \text{for } |\mathbf{x}| \geq R_0, \end{cases} \quad (2-28)$$

for some $C_0 > 0$. The first two equations in (2-28) are consequences of the last equation in (2-27) and the definition of the coincident set Ω_∞ with $|\partial\Omega_\infty| = 0$. To justify the last equation, we notice that, by the maximum principle applied to the first of (2-23), the minimum of $u_r(\mathbf{x})$ must be attained at ∂B_r which implies $u_r(\mathbf{x}) \geq 0$ on B_r . It then follows that the coincident set Ω_r is contained in the open ball B_{R_0} for all $r > R_0$. Then it can be verified, by the method of Green's functions (GILBARG & TRUDINGER [17], page 19), that for $n \geq 3$

$$|u_r(\mathbf{x})| \leq \frac{C_0}{|\mathbf{x}|^{n-2}} \quad \forall R_0 \leq |\mathbf{x}| < r, \quad (2-29)$$

where C_0 is a positive constant independent of r . Therefore, by the triangle inequality, $|u_\infty| \leq |u_{r_j} - u_\infty| + |u_{r_j}| \leq |u_{r_j} - u_\infty| + C_0/|\mathbf{x}|^{n-2}$ on B_R . Fixing R and taking the limsup over $r_j > R$ we get the desired result.

Finally we show the limiting minimizer u_∞ must be unique and the convergence in equation (2-26) is in fact strong. Assume there is a second limit u'_∞ that satisfies (2-26), and therefore, (2-27)-(2-28). Equations (2-27) and (2-28) imply that for any $v \in K_\infty := \{u \in W_{loc}^{1,2}(\mathbb{R}^n) : u \geq \phi, \int_{\mathbb{R}^n} |\nabla u|^2 d\mathbf{x} < \infty, |u(\mathbf{x})| \rightarrow 0 \text{ as } |\mathbf{x}| \rightarrow \infty\}$,

$$\begin{aligned} \int_{\mathbb{R}^n} \nabla u_\infty \cdot \nabla(v - u_\infty) d\mathbf{x} &= \int_{\mathbb{R}^n} (-\Delta u_\infty)(v - u_\infty) d\mathbf{x} \\ &= \int_{\{u_\infty > \phi\}} (-\Delta u_\infty)(v - u_\infty) d\mathbf{x} + \int_{\{u_\infty = \phi\}} (-\Delta u_\infty)(v - \phi) d\mathbf{x} \geq 0. \end{aligned} \quad (2-30)$$

Clearly, equation (2-30) holds with u_∞ replaced by u'_∞ as well:

$$\int_{\mathbb{R}^n} \nabla u'_\infty \cdot \nabla(v - u'_\infty) d\mathbf{x} \geq 0 \quad \forall v \in K_\infty. \quad (2-31)$$

Since $u'_\infty, u_\infty \in K_\infty$, adding equation (2-30) with $v = u'_\infty$ to equation (2-31) with $v = u_\infty$, we obtain

$$-\int_{\mathbb{R}^n} |\nabla(u'_\infty - u_\infty)|^2 d\mathbf{x} \geq 0.$$

Thus, u_∞ can be different from u'_∞ at most by a constant. From the last equation in (2-28) it follows that $u'_\infty = u_\infty$.

We summarize below.

Theorem 5. *Consider the variational inequality problem (2-20) with a piecewise quadratic obstacle ϕ and define the limiting minimizer u_∞ and coincident set Ω_∞ as above. Then, the coincident set Ω_∞ is an E -inclusion.*

We remark that the Eshelby conjectures (ESHELBY [12]) can be proved in the framework of variational inequalities. The details will be presented in a separate publication (LIU [36]). Recently we learned of that KANG & MILTON [26] independently proved these conjectures, who also observed that the Pólya-Szegő conjecture (PÓLYA & SZEGŐ [48]) is equivalent to a version of the Eshelby conjectures.

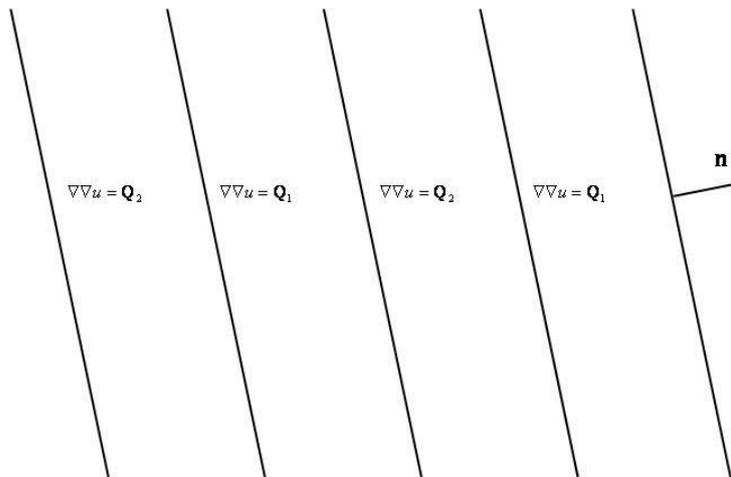


Fig. 1. Simple laminations belong to a special family of periodic E -inclusions.

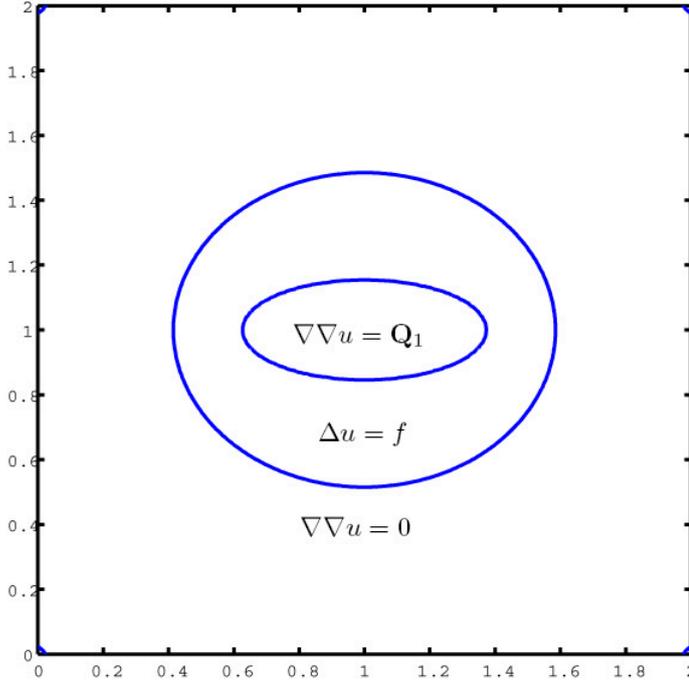


Fig. 2. *Confocal ellipses are a special family of periodic E-inclusions.*

3. Examples of periodic E-inclusions

We now consider various examples of periodic E-inclusions. From the discussion above, periodic E-inclusions constructed by Theorem 2 can be specified by a Bravais lattice \mathcal{L} , the quantity $f > 0$ and a periodic piecewise quadratic obstacle ϕ_{per} . It is worthwhile noticing that from the comparison theorem (see e.g. FRIEDMAN [15], page 26), periodic E-inclusions corresponding to a fixed obstacle satisfy $\Omega_{per}^{f_1} \subset \Omega_{per}^{f_2}$ if $f_2 > f_1 > 0$. Also the interior of any periodic E-inclusion cannot contain the singular points of the obstacle on which $\nabla\nabla\phi_{per}$ is unbounded in distributional sense. By varying the obstacle ϕ_{per} and f , a large class of periodic E-inclusions can be constructed in any dimension $n \geq 1$. We show a few examples of them below.

The first example is a simple lamination. Let $\mathbf{n} \in \mathbb{R}^n$ be a unit vector, $f > 0$, $a < 0$, and $h_{per}(x) = \max\{\frac{1}{2}a(x+\nu)^2 : \nu \in \mathbb{Z}\}$ for $x \in \mathbb{R}$. Consider the obstacle

$$\phi_{per}(\mathbf{x}) = h_{per}(\mathbf{x} \cdot \mathbf{n}).$$

By the method given above this is a periodic E-inclusion corresponding to $\mathbf{Q}_1 = a\mathbf{n} \otimes \mathbf{n}$ and $\mathbf{Q}_2 = f\mathbf{n} \otimes \mathbf{n}$ with volume fractions $f/(f-a)$ and $-a/(f-a)$, respectively, see Fig. 1. In another words a simple lamination is a periodic E-inclusion.

The coated spheres (HASHIN & SHTRIKMAN [21]) and confocal ellipsoids (MILTON [42]), familiar from homogenization theory, can be constructed as a periodic E-inclusions. The example in Fig. 2 is computed by using the obstacle

$$\phi_{per}(\mathbf{x}) = \max\{0, \frac{1}{2}(\mathbf{x} + \mathbf{r}) \cdot \mathbf{Q}_1(\mathbf{x} + \mathbf{r}) + h_1 : \mathbf{r} \in \mathcal{L}\},$$

where $h_1 > 0$, $\mathbf{Q}_1 < 0$ are appropriately chosen so that the graph of the obstacle consists of isolated “mountains” emerging out of a horizontal “sea”. So, if f is large enough, the minimizer u_f contacts the mountains around the peaks and the sea but is detached from the rim of singular points of ϕ_{per} . It can be proved that the coincident set in each unit cell is separated by two confocal ellipsoids, by noticing the Newtonian potential of a homogeneous solid ellipsoid is not only quadratic inside the ellipsoid, but also quadratic outside the ellipsoid on the equipotential surface which is a confocal ellipsoid, see KELLOGG [28]. On the other hand, if f is very small or the obstacles of (2-8) are considered, one obtains the Vigdergauz-type structure as the coincident set of the variational inequality (2-1); see also GRABOVSKY & KOHN [20] for an analytic derivation of the Vigdergauz structure. Our constructions generalize immediately to higher dimensions.

More general periodic E-inclusions are not amenable to simple analytic descriptions. So we turn to numerical methods, which are easy to implement for the variational inequality. First let us consider the variational problem (2-1) with the constraint $u \geq \phi_{per}$ neglected. Clearly the Euler-Lagrange equation of this variational problem is the Poisson equation

$$\begin{cases} \Delta u = f & \text{on } Y, \\ \text{periodic boundary conditions} & \text{on } \partial Y, \end{cases}$$

which, according to the finite element method (see e.g. KWON & BANG [34]), can be discretized as

$$\hat{K}\hat{u} = \hat{f}. \quad (3-1)$$

Here \hat{u} , a column vector, denotes the values of the potential u at the nodal points in the finite element model, \hat{K} and \hat{f} are usually called the *stiffness matrix* and *loads*, respectively. Now let us take into account the discretized constraint $\hat{u} \geq \hat{\phi}_{per}$, where $\hat{\phi}_{per}$ are the values of the obstacle $\hat{\phi}_{per}$ at the nodal points. The discrete version of the variational inequality (2-1) becomes the following quadratic programming problem:

$$\min\{\hat{G}(\hat{u}) = -\frac{1}{2}\hat{u} \cdot \hat{K}\hat{u} + \hat{f} \cdot \hat{u} : \hat{u} \geq \hat{\phi}_{per}\}, \quad (3-2)$$

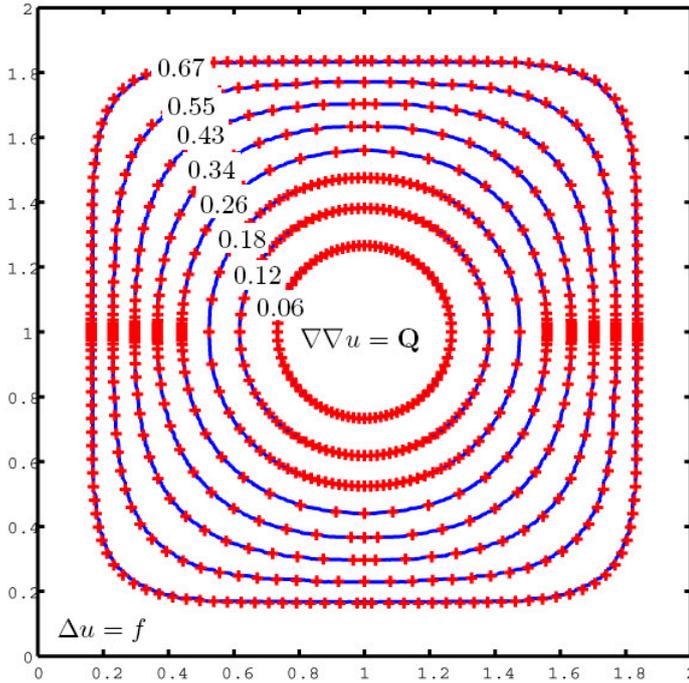


Fig. 3. *Vigdergauz structures in a square cell corresponding to $\mathbf{Q} = -\text{diag}(1, 1)$. The blue curves are our numerical results based on the variational inequality, and the red “+” signs are the analytic solutions. The inset numbers are the volume fractions of the Vigdergauz structures.*

which can be easily solved using standard solvers. The following computations use a uniform mesh with around 10^5 nodal points. The iterations are terminated when the relative difference between the values $\hat{G}(\hat{u})$ of two consecutive iterations is less than 10^{-10} . With these parameters, the iterations converge within a few minutes on a personal computer. The resulting periodic E-inclusion includes all nodal points on which $|\hat{u} - \hat{\phi}|$ is less than $a \times 10^{-3}$, where a is at the order of 1.

The numerical scheme is verified by comparing the results with the analytic solutions for the Vigdergauz structures in two dimensions with a square unit cell and with $\mathbf{Q} = -\text{diag}(1, 1)$. The volume fractions were chosen to be, from inward to outward, 0.06, 0.12, 0.18, 0.26, 0.34, 0.43, 0.55, 0.67. In Fig. 3 the solid blue curves are the numerical results while the red “+” signs denote the analytic solutions. There is good agreement between the exact shapes and our calculated shapes. As is well-known from the Vigdergauz construction, E-inclusions are asymptotic to a circle at small volume fraction and to the unit square at volume fractions approaching one.

It should be noticed that a periodic E-inclusion may not look like an “inclusion” at all. Figure 2 shows such an example, the E-inclusion being

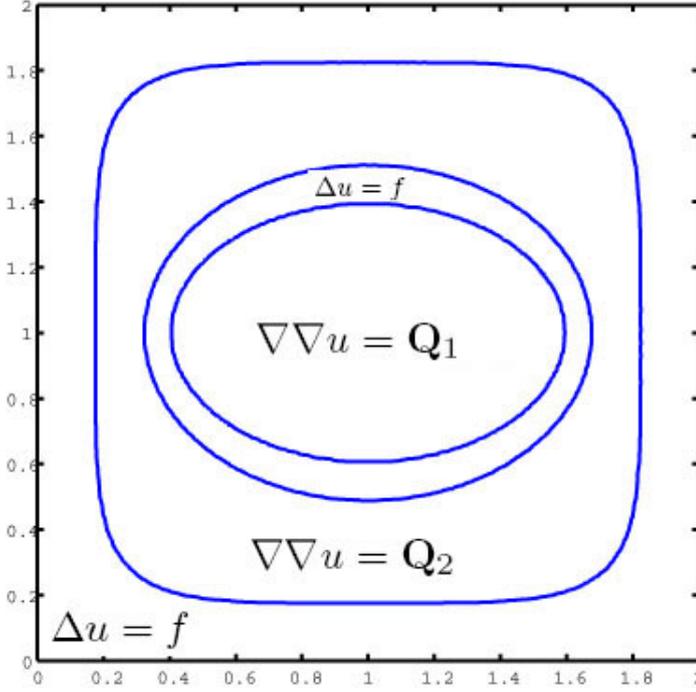


Fig. 4. A periodic E -inclusion in the case $N = 2$ with two components corresponding to $\mathbf{Q}_1 = -\text{diag}(1, 1)$ and $\mathbf{Q}_2 = -\text{diag}(2, 3)$, and volume fractions 0.19 and 0.65, respectively.

the interior of the inner ellipse and the exterior of the outer ellipse. A more general example is shown in Fig. 4. This example is calculated using the obstacle

$$\phi_{per}(\mathbf{x}) = \max\left\{\frac{1}{2}(\mathbf{x} + \mathbf{r}) \cdot \mathbf{Q}_1(\mathbf{x} + \mathbf{r}), \frac{1}{2}(\mathbf{x} + \mathbf{r}) \cdot \mathbf{Q}_2(\mathbf{x} + \mathbf{r}) + h_2 : \mathbf{r} \in 2\mathbb{Z}^2 - \mathbf{d}\right\},$$

where

$$\mathbf{Q}_1 = -\text{diag}(1, 1), \quad \mathbf{Q}_2 = -\text{diag}(2, 3), \quad \mathbf{d} = (1, 1) \quad \text{and} \quad h_2 = 0.2.$$

The periodic E -inclusion has two components: one consists of the inner region corresponding to \mathbf{Q}_1 and volume fraction 0.19, and the other is the squarish annulus corresponding to \mathbf{Q}_2 and volume fraction 0.65. This type of structure can be regarded as a generalization of multi-coated spheres (LURIE & CHERKAEV [40]) in the periodic setting.

An interesting scenario is plotted in Fig. 5. Periodic E -inclusions in this figure, corresponding to two different matrices \mathbf{Q}_1 and \mathbf{Q}_2 , have nevertheless

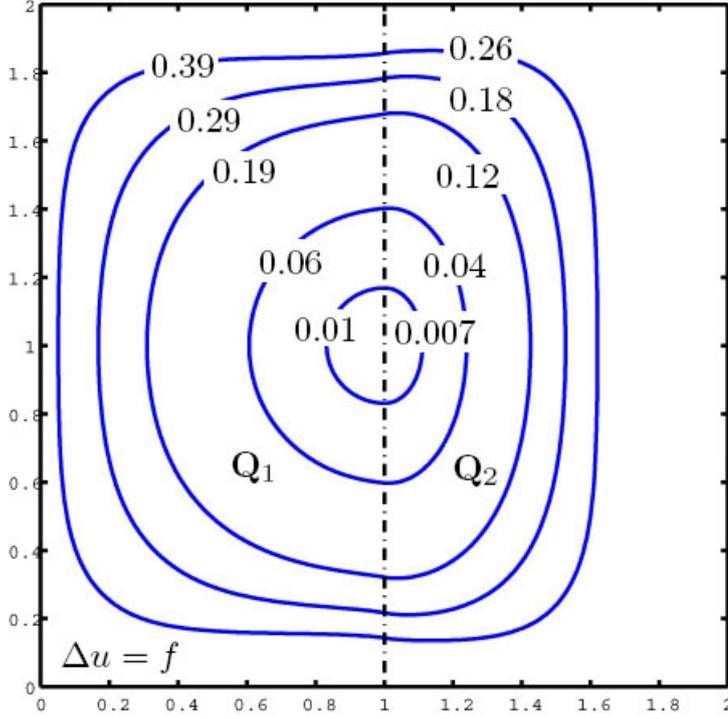


Fig. 5. A sequence of periodic E -inclusions with $N = 2$, $\mathbf{Q}_1 = -\text{diag}(1, 1)$ and $\mathbf{Q}_2 = -\text{diag}(2, 1)$. In this case \mathbf{Q}_1 and \mathbf{Q}_2 differ by a rank-one matrix and the two parts of E -inclusion are separated by a plane. The volume fractions from inward to outward are $(0.01, 0.007)$, $(0.06, 0.04)$, $(0.19, 0.12)$, $(0.29, 0.18)$, $(0.39, 0.26)$.

only one connected component in one unit cell. Periodic E -inclusions of this kind can be constructed by using the obstacle

$$\phi_{per}(\mathbf{x}) = \max\{P(\mathbf{x} + \mathbf{r}) : \mathbf{r} \in \mathcal{L}\},$$

where

$$P(\mathbf{x}) = \begin{cases} \frac{1}{2}\mathbf{x} \cdot \mathbf{Q}_1\mathbf{x} & \text{if } \mathbf{x} \cdot \mathbf{n} < 0, \\ \frac{1}{2}\mathbf{x} \cdot \mathbf{Q}_2\mathbf{x} & \text{if } \mathbf{x} \cdot \mathbf{n} \geq 0, \end{cases}$$

$\mathbf{Q}_1, \mathbf{Q}_2 < 0$ and $\mathbf{Q}_1 - \mathbf{Q}_2 = b\mathbf{n} \otimes \mathbf{n}$ for some $b \in \mathbb{R}$ and unit vector $\mathbf{n} \in \mathbb{R}^n$. Inside such a periodic E -inclusion, there is a plane interface with normal \mathbf{n} that separates $\nabla\nabla u = \mathbf{Q}_1$ and $\nabla\nabla u = \mathbf{Q}_2$. Figure 5 is plotted by using

$$\mathbf{Q}_1 = -\text{diag}(1, 1) \quad \text{and} \quad \mathbf{Q}_2 = -\text{diag}(2, 1).$$

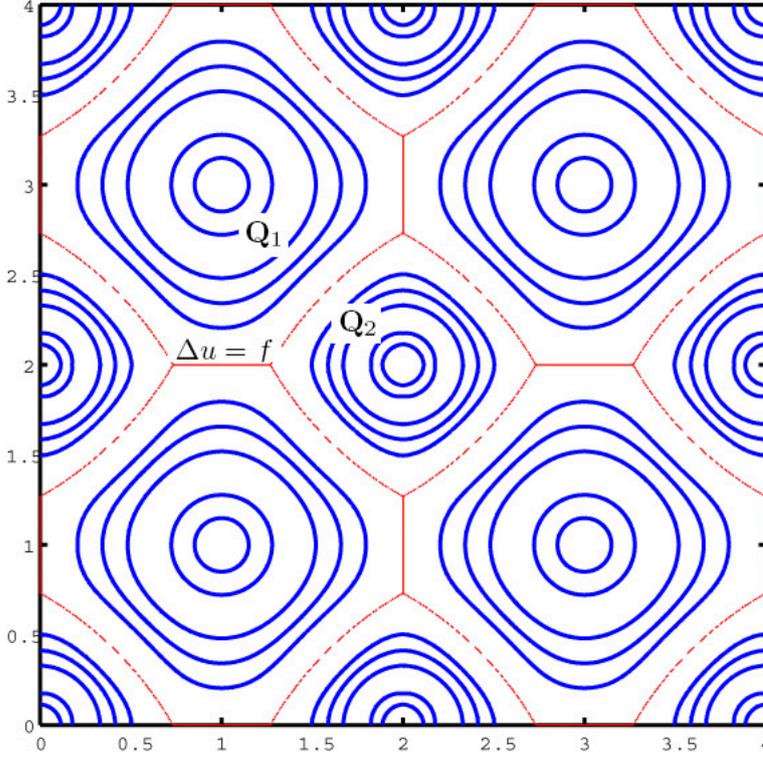


Fig. 6. A sequence of periodic E-inclusions with $N = 2$, $\mathbf{Q}_1 = -\text{diag}(1, 1)$ and $\mathbf{Q}_2 = -\text{diag}(2, 2)$. The volume fractions from inward to outward are $(0.02, 0.01)$, $(0.07, 0.03)$, $(0.22, 0.09)$, $(0.33, 0.14)$, $(0.45, 0.19)$. The figure shows four unit cells.

The periodic E-inclusions corresponding to $(\mathbf{Q}_1, \mathbf{Q}_2)$, from inward to outward, have volume fractions $(0.01, 0.007)$, $(0.06, 0.04)$, $(0.19, 0.12)$, $(0.29, 0.18)$, $(0.39, 0.26)$.

We can construct periodic E-inclusions with multiple components of a very different topology from Fig. 4. Consider the obstacle

$$\phi_{per}(\mathbf{x}) = \max\left\{\frac{1}{2}(\mathbf{x} - \mathbf{d}_i + \mathbf{r}) \cdot \mathbf{Q}_i(\mathbf{x} - \mathbf{d}_i + \mathbf{r}) : \right. \\ \left. i = 1, \dots, N; \mathbf{r} \in \mathcal{L}\right\}, \quad (3-3)$$

where $\mathbf{d}_1, \dots, \mathbf{d}_N \in \mathbb{R}^n$. Figure 6 shows examples of this kind, corresponding to $\mathcal{L} = 2\mathbb{Z}^2$, $N = 2$, and

$$\mathbf{Q}_1 = -\text{diag}(1, 1), \quad \mathbf{Q}_2 = -\text{diag}(2, 2), \quad \mathbf{d}_1 = [1, 1], \quad \mathbf{d}_2 = [2, 2].$$

Note that four unit cells are plotted in the figure. Each periodic E-inclusion has two components in one unit cell corresponding to \mathbf{Q}_1 and \mathbf{Q}_2 , respec-

tively. The volume fractions, from inward to outward, are (0.02, 0.01), (0.07, 0.03), (0.22, 0.09), (0.33, 0.14), (0.45, 0.19). The red curves delimit the singular points of the obstacle which can never intersect the interior of an E-inclusion. Thus, the boundaries of the E-inclusions approach the red curves since the total volume fractions of the E-inclusions approach 1 as $f \rightarrow +\infty$, as is implied by equation (2-13).

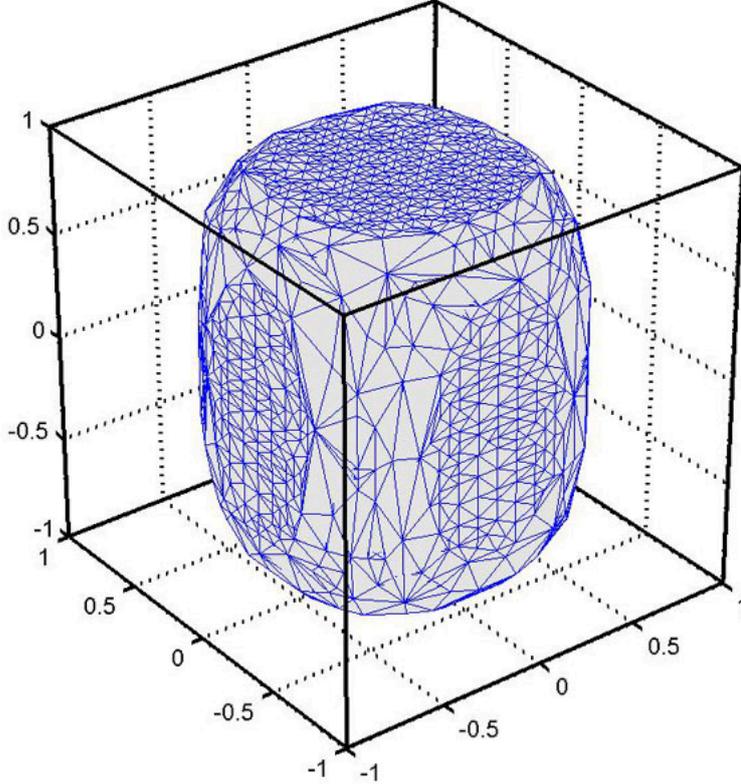


Fig. 7. A periodic E-inclusion corresponding to $N = 1$, $\mathbf{Q}_1 = \mathbf{Q} = -\text{diag}(3, 3, 1)$, and volume fraction 0.37.

The numerical scheme (3-1) can also be carried out in three dimensions. The meshes used in three dimensions are not as dense as those in two dimensions. So, the computed E-inclusions are less smooth than those in two dimensions. Simplified computations have been performed and approximate periodic 3-D E-inclusions with cubic symmetry have been given in LIU, JAMES & LEO [38]. There it was noted that the periodic E-inclusions are well approximated by *generalized ellipsoids* defined by

$$GE(\alpha) = \{(x_1, x_2, x_3) : \frac{x_1^\alpha}{a_1^\alpha} + \frac{x_2^\alpha}{a_2^\alpha} + \frac{x_3^\alpha}{a_3^\alpha} \leq 1\}.$$

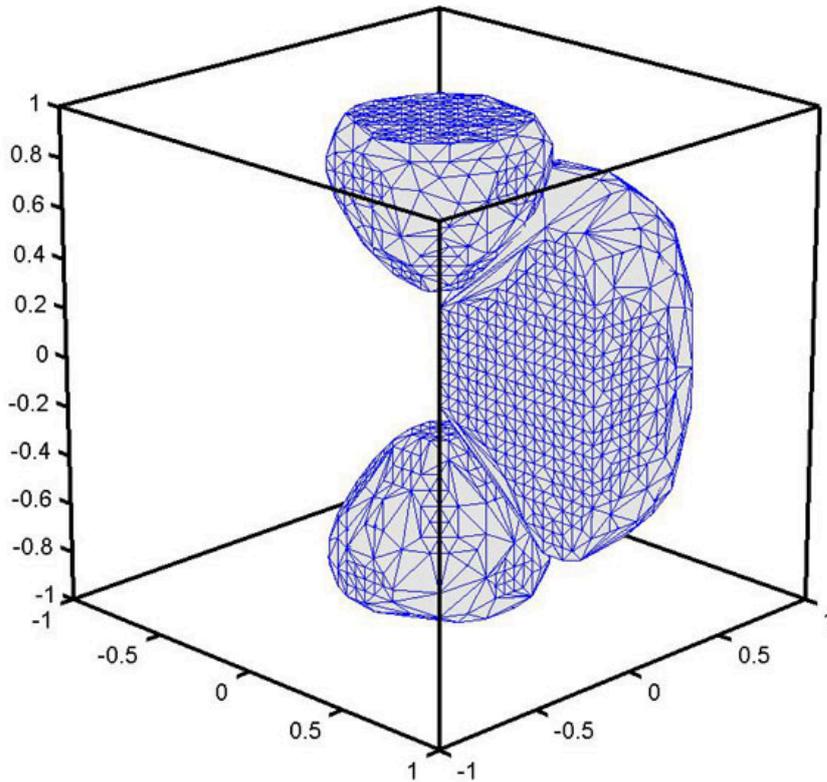


Fig. 8. A periodic E -inclusion with $N = 3$ having three components in the unit cell and $\mathbf{Q}_1 = -\text{diag}(1, 1, 1)$, $\mathbf{Q}_2 = \mathbf{Q}_3 = -\text{diag}(3, 3, 1)$. The top and bottom components corresponding to \mathbf{Q}_2 and \mathbf{Q}_3 are mirror symmetric and have the same volume fraction 0.03, and the middle component has volume fraction 0.35. Only one fourth of the middle component is plotted in the figure. The full middle component is shown separately in Fig. 9

We then optimized the index α such that $GE(\alpha)$ is the best approximation according to certain criterion. This formula can interpolate an ellipsoid and a cube. In present approach no assumption are made about the shape of the E -inclusions to be calculated.

Not surprisingly, the different scenarios represented in figures 1-6 are all realizable in three dimensions. Three typical examples are selected here. In Fig. 7 a periodic E -inclusion is calculated in the cubic unit cell $(-1, 1)^3$ with the obstacle (2-8) and $\mathbf{Q} = -\text{diag}(3, 3, 1)$. The volume fraction of this E -inclusion is 0.37. The tendency of the boundaries of the E -inclusion to become flatter when they come closer to each other is more obvious in three

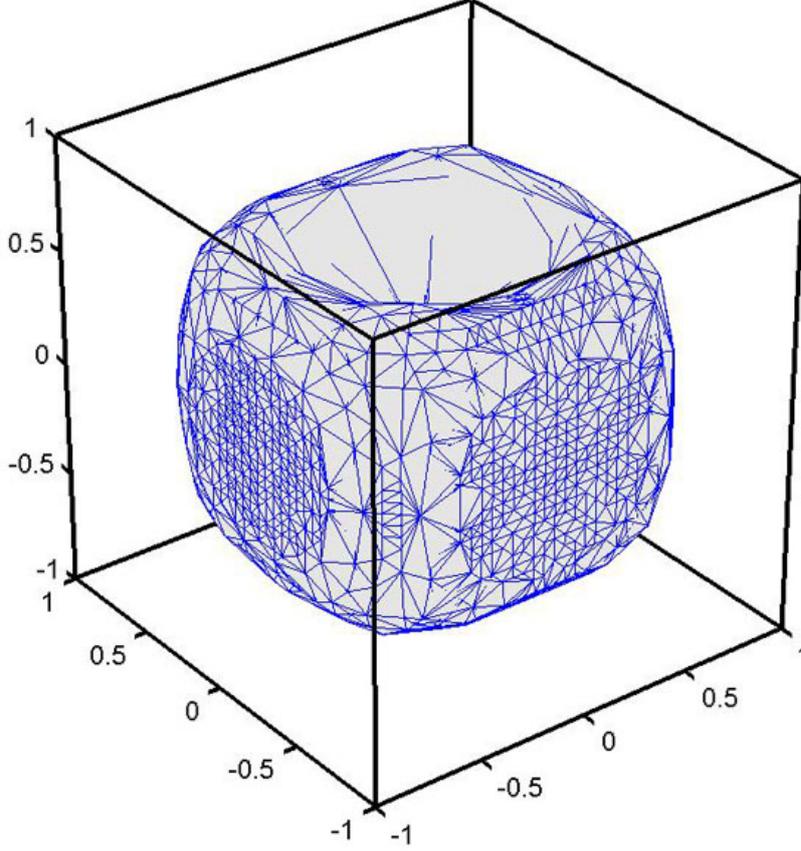


Fig. 9. The middle component of the periodic E-inclusion in Fig. 8 shown separately.

dimensions. The mesh in this and following figures does not represent the actual mesh used in the computation but is merely used for visualization.

A three-component periodic E-inclusion is plotted in Fig. 8. It is calculated using the obstacle

$$\phi_{per}(\mathbf{x}) = \max\left\{\frac{1}{2}(\mathbf{x} + \mathbf{r} + \mathbf{d}_i) \cdot \mathbf{Q}_i(\mathbf{x} + \mathbf{r} + \mathbf{d}_i) : i = 1, 2, 3, \mathbf{r} \in 2\mathbb{Z}^3\right\},$$

where $\mathbf{Q}_1 = -\text{diag}(1, 1, 1)$, $\mathbf{Q}_2 = \mathbf{Q}_3 = -\text{diag}(3, 3, 1)$, $\mathbf{d}_1 = (0, 0, 0)$, $\mathbf{d}_2 = (0, 0, 0.5)$ and $\mathbf{d}_3 = (0, 0, -0.5)$. The top and bottom components corresponding to $(\mathbf{Q}_2, \mathbf{Q}_3)$ have the same volume fraction 0.03 and the middle component corresponding to \mathbf{Q}_1 has volume fraction 0.35. Note that only one fourth of the middle component is plotted in Fig. 8. The middle component is plotted separately in Fig. 9. A final example is shown in

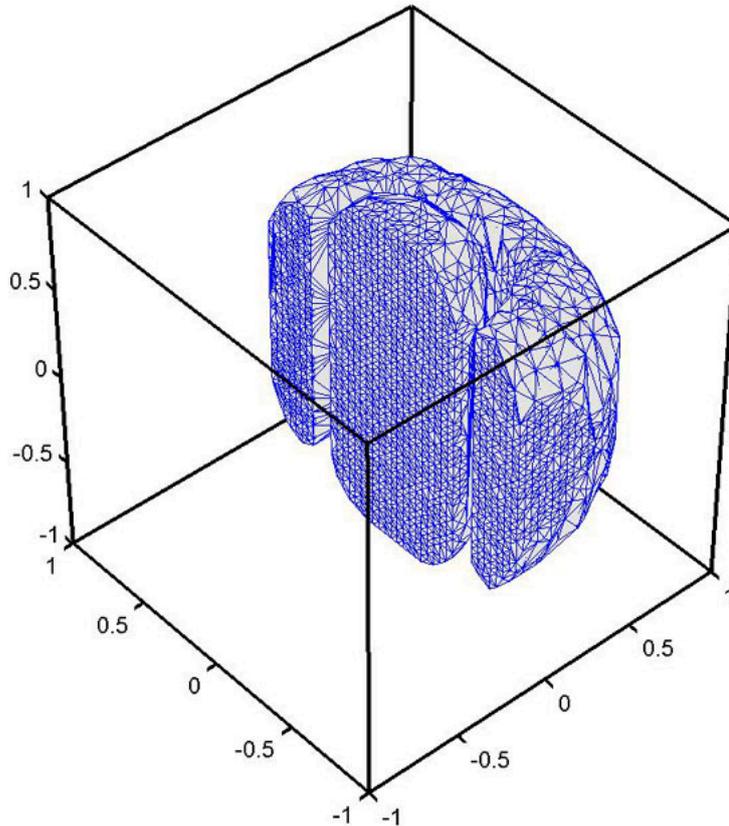


Fig. 10. A periodic E-inclusion for the case $N = 2$ with one component surrounding the other in the unit cell. Only half of the E-inclusion is shown. The inner and outer components correspond to matrices $\mathbf{Q}_2 = -\text{diag}(3, 3, 1)$, $\mathbf{Q}_1 = -\text{diag}(1, 1, 1)$ and have volume fractions $(0.11, 0.40)$, respectively. See Fig. 11 for top view.

Fig. 10, which is calculated with the obstacle

$$\phi_{per}(\mathbf{x}) = \max\left\{\frac{1}{2}(\mathbf{x} + \mathbf{r}) \cdot \mathbf{Q}_1(\mathbf{x} + \mathbf{r}), \frac{1}{2}(\mathbf{x} + \mathbf{r}) \cdot \mathbf{Q}_2(\mathbf{x} + \mathbf{r}) + h_2 : \mathbf{r} \in 2\mathbb{Z}^3\right\},$$

where $\mathbf{Q}_1 = -\text{diag}(1, 1, 1)$, $h_2 = 0.2$ and $\mathbf{Q}_2 = -\text{diag}(3, 3, 1)$. Only half of the E-inclusion is plotted in this figure. The inner and outer components in the figure correspond to $(\mathbf{Q}_2, \mathbf{Q}_1)$ and have volume fractions $(0.11, 0.40)$, respectively. The top view is shown in Fig. 11.

4. Applications

In this section, we use periodic E-inclusions to solve problems for two-phase composites. From Definition 1 a periodic E-inclusion is associated to

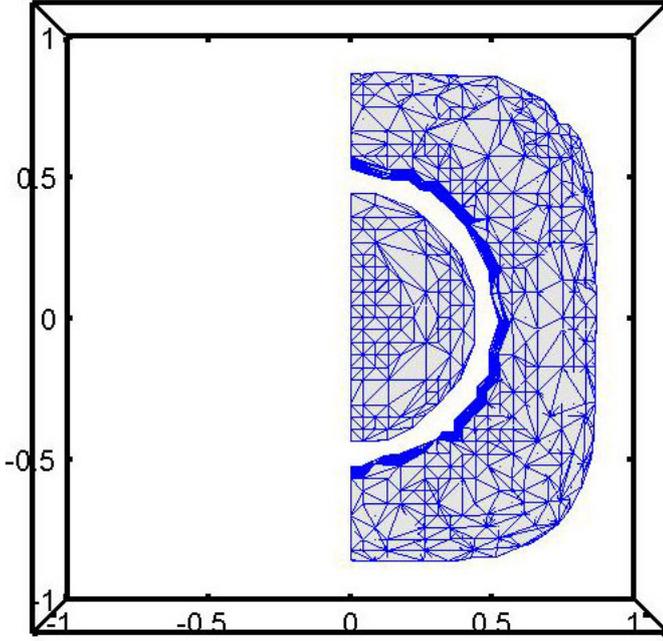


Fig. 11. Top view of the periodic E-inclusion in Fig. 10. As in Fig. 10 only half of the inclusion is shown.

matrices \mathbb{K} and volume fractions Θ . In general periodic E-inclusions having $N' \leq N$ distinct matrices in \mathbb{K} can be used to solve problems for $(N' + 1)$ -phase composites. For two-phase composites we need only periodic E-inclusions with $\mathbb{K} = \{\mathbf{Q}, \mathbf{Q}, \dots, \mathbf{Q}\}$. Applications of periodic E-inclusions to multi-phase composites are presented in a separate publication (LIU [35]).

4.1. Periodic Eshelby inclusion problems and effective properties of two-phase composites

Our first observation is that some effective properties of composites having one phase made with periodic E-inclusions can be easily calculated. We consider a periodic two-phase composite defined by

$$\mathbf{L}(\mathbf{x}, \Omega) = \begin{cases} \mathbf{L}_1 \in \mathbb{L} & \mathbf{x} \in \Omega, \\ \mathbf{L}_2 \in \mathbb{L} & \mathbf{x} \in Y \setminus \Omega, \end{cases} \quad (4-1)$$

where the notation is as above, $\Omega \subset Y$ is measurable, $Y \subset \mathbb{R}^n$ is an open unit cell, and the set \mathbb{L} is the collection of all self-adjoint linear mappings $\hat{\mathbf{L}} : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}^{m \times n}$ that satisfy

$$\hat{\mathbf{L}} > 0 \quad \text{or} \\ X \cdot \hat{\mathbf{L}}X > 0 \quad \forall X^T = X \neq 0 \quad \text{and} \quad X \cdot \hat{\mathbf{L}}X = 0 \quad \forall X^T = -X. \quad (4-2)$$

Note that \mathbf{L}_1 and \mathbf{L}_2 need not satisfy the full symmetries of linear elasticity tensors. The benefit of this general setting is that several problems including the conductivity problem can be treated simultaneously. Throughout this section the periodicity and unit cell Y are fixed.

Consider the minimization problem

$$J_*(\mathbf{L}, \mathbf{F}, \Omega) = \min \left\{ \frac{1}{2} \int_Y (\nabla \mathbf{v} + \mathbf{F}) \cdot \mathbf{L}(\mathbf{x}, \Omega) (\nabla \mathbf{v} + \mathbf{F}) d\mathbf{x} : \right. \quad (4-3)$$

$$\left. \mathbf{v} \in W_{per}^{1,2}(Y; \mathbb{R}^m) \right\}.$$

Physically, in the case of linearized elasticity $J_*(\mathbf{L}, \mathbf{F}, \Omega)$ is the elastic energy density induced by an applied average strain $\mathbf{F} \in \mathbb{R}^{m \times n}$. The effective tensor $\mathbf{L}^e(\Omega)$ is defined as (CHRISTENSEN [8])

$$\frac{1}{2} \mathbf{F} \cdot \mathbf{L}^e(\Omega) \mathbf{F} = J_*(\mathbf{L}, \mathbf{F}, \Omega) \quad \forall \mathbf{F} \in \mathbb{R}^{m \times n}. \quad (4-4)$$

From standard arguments in the calculus of variations (EVANS [14]), a minimizer of problem (4-3) exists and necessarily satisfies the Euler-Lagrange equation

$$\begin{cases} \operatorname{div} [\mathbf{L}(\mathbf{x}, \Omega) (\nabla \mathbf{v} + \mathbf{F})] = 0 & \text{on } Y, \\ \text{periodic boundary conditions} & \text{on } \partial Y. \end{cases} \quad (4-5)$$

We are interested in calculating the effective tensor $\mathbf{L}^e(\Omega)$. Problem (4-5) is referred to as the *inhomogeneous* Eshelby inclusion problem in a periodic setting (cf., equation (1-2)).

The relation between periodic E-inclusions and problem (4-5) can be uncovered by adapting a well-known argument of ESHELBY [13]. We begin with the *homogeneous* Eshelby inclusion problem,

$$\begin{cases} \operatorname{div} [\mathbf{L}_2 \nabla \mathbf{v} + \mathbf{P} \chi_\Omega] = 0 & \text{on } Y, \\ \text{periodic boundary conditions} & \text{on } \partial Y, \end{cases} \quad (4-6)$$

where $\mathbf{P} \in \mathbb{R}^{m \times n}$ is given and $\mathbf{v} \in W_{per}^{1,2}(Y, \mathbb{R}^m)$ is the unknown. Below, we sometimes write $\mathbf{v}(\mathbf{x}, \mathbf{P})$ to emphasize the (linear) dependence of \mathbf{v} on \mathbf{P} . Further, motivated by the convenient property of ellipsoids employed by Eshelby, we assume that Ω and \mathbf{P} are such that there is a solution \mathbf{v} of the homogeneous problem (4-6) satisfying

$$\nabla \mathbf{v}(\mathbf{x}, \mathbf{P}) = -(1 - \theta) \mathbf{R} \mathbf{P} \quad \text{on } \Omega, \quad (4-7)$$

where $\theta = |\Omega|/|Y|$ is the volume fraction of the inclusion, and the linear mapping

$$\mathbf{R} \mathbf{P} = \frac{-1}{1 - \theta} \int_\Omega \nabla \mathbf{v}(\mathbf{x}, \mathbf{P}) d\mathbf{x} \quad (4-8)$$

is self-adjoint and depends on Ω (for the self-adjointness, see equation (4-30)). From equations (4-6) and (4-8), it follows that

$$\int_Y \nabla \mathbf{v}(\mathbf{x}, \mathbf{P}) \cdot \mathbf{L}_2 \nabla \mathbf{v}(\mathbf{x}, \mathbf{P}) d\mathbf{x} = \theta(1 - \theta) \mathbf{P} \cdot \mathbf{R} \mathbf{P} \geq 0 \quad \forall \mathbf{P} \in \mathbb{R}^{m \times n}. \quad (4-9)$$

Together with equation (4-7) and following the Eshelby's argument, we now observe that a solution of problem (4-6) also solves problem (4-5) under restrictions given below. To see this, let us formally rewrite equations (4-6) and (4-5) in a less concise form as

$$\begin{cases} \operatorname{div}[\mathbf{L}_2 \nabla \mathbf{v}] = 0 & \text{in } Y \setminus \Omega, \\ \operatorname{div}[\mathbf{L}_2 \nabla \mathbf{v}] = 0 & \text{in } \Omega, \\ \llbracket \mathbf{L}_2 \nabla \mathbf{v} + \mathbf{P} \chi_{\Omega} \rrbracket \mathbf{n} = 0 & \text{on } \partial \Omega, \end{cases} \quad (4-10)$$

and

$$\begin{cases} \operatorname{div}[\mathbf{L}_2 \nabla \mathbf{v}] = 0 & \text{in } Y \setminus \Omega, \\ \operatorname{div}[\mathbf{L}_1 \nabla \mathbf{v}] = 0 & \text{in } \Omega, \\ \llbracket \mathbf{L}(\mathbf{x}, \Omega)(\nabla \mathbf{v} + \mathbf{F}) \rrbracket \mathbf{n} = 0 & \text{on } \partial \Omega, \end{cases} \quad (4-11)$$

respectively, where $\llbracket \cdot \rrbracket$ denotes the jump across the $\partial \Omega$. By matching the jump conditions in (4-10) and (4-11), direct calculations show that if \mathbf{v} satisfies all equations in (4-10) and equation (4-7), then \mathbf{v} also satisfies all equations in (4-11) for \mathbf{F} satisfying

$$\Delta \mathbf{L} \mathbf{F} = (1 - \theta) \Delta \mathbf{L} \mathbf{R} \mathbf{P} - \mathbf{P}, \quad (4-12)$$

where $\Delta \mathbf{L} = \mathbf{L}_2 - \mathbf{L}_1$. Properly interpreted, this formal argument can be made rigorous. More specifically, the weak form of (4-6) is

$$\int_Y (\mathbf{L}_2 \nabla \mathbf{v} + \mathbf{P} \chi_{\Omega}) \cdot \nabla \mathbf{w} d\mathbf{x} = 0 \quad \forall \mathbf{w} \in W_{per}^{1,2}(Y; \mathbb{R}^m). \quad (4-13)$$

By equations (4-7) and (4-12), equation (4-13) can be rewritten as

$$\int_Y [\mathbf{L}_2 \nabla \mathbf{v} - \Delta \mathbf{L}(\nabla \mathbf{v} + \mathbf{F}) \chi_{\Omega}] \cdot \nabla \mathbf{w} d\mathbf{x} = 0 \quad \forall \mathbf{w} \in W_{per}^{1,2}(Y; \mathbb{R}^m),$$

which is exactly the weak form of (4-5). Also, the energy of the inhomogeneous problem (4-5) can be conveniently written as

$$\begin{aligned} 2J_*(\mathbf{L}, \mathbf{F}, \Omega) &= \int_Y (\nabla \mathbf{v} + \mathbf{F}) \cdot \mathbf{L}(\mathbf{x}, \Omega)(\nabla \mathbf{v} + \mathbf{F}) d\mathbf{x} \\ &= \int_Y \mathbf{F} \cdot \mathbf{L}(\mathbf{x}, \Omega)(\nabla \mathbf{v} + \mathbf{F}) d\mathbf{x} \\ &= \int_Y \mathbf{F} \cdot \mathbf{L}_2 \mathbf{F} d\mathbf{x} - \int_Y \mathbf{F} \cdot \Delta \mathbf{L}(\nabla \mathbf{v} + \mathbf{F}) \chi_{\Omega} d\mathbf{x} \\ &= \mathbf{F} \cdot \mathbf{L}_2 \mathbf{F} + \theta \mathbf{P} \cdot \mathbf{F}, \end{aligned} \quad (4-14)$$

where \mathbf{F} and \mathbf{P} are related by equation (4-12).

As emphasized above, equation (4-7) is not true unless the inclusion Ω is very special. We now show that periodic E-inclusions given by Theorem 3 are indeed such special inclusions in many interesting situations. First we explain the relation between the scalar and vector-valued problems.

Lemma 1. *Let $u \in W_{per}^{2,2}(Y)$ be a solution of problem*

$$\begin{cases} \Delta u = \theta - \chi_\Omega & \text{on } Y, \\ \text{periodic boundary conditions} & \text{on } \partial Y. \end{cases} \quad (4-15)$$

Denote by δ_{ij} ($i, j = 1, \dots, n$) the components of the identity matrix $\mathbf{I} \in \mathbb{R}^{n \times n}$. If $m = n \geq 1$, $\mathbf{L}_2 \in \mathbb{L}$ (cf., (4-2)), and

$$(\mathbf{L}_2)_{piqj} = \mu_1 \delta_{ij} \delta_{pq} + \mu_2 \delta_{pj} \delta_{iq} + \lambda \delta_{ip} \delta_{jq}, \quad (4-16)$$

then

$$\mathbf{v}(\mathbf{x}, \mathbf{P}) = \frac{\mathbf{P} \nabla u(\mathbf{x})}{\lambda + \mu_1 + \mu_2} \quad (4-17)$$

solves problem (4-6) for $\mathbf{P} = \mathbf{I}$. If $\mu_2 + \lambda = 0$ then \mathbf{v} defined by (4-17) solves problem (4-6) for every $\mathbf{P} \in \mathbb{R}^{n \times n}$.

Proof. Note that $\mathbf{L}_2 \in \mathbb{L}$ implies the constants μ_1 , μ_2 and λ necessarily satisfy $\mu_1 \geq \mu_2$, $\mu_1 + \mu_2 > 0$ and $\lambda > -\frac{\mu_1 + \mu_2}{n}$. Since $(\mathbf{L}_2)_{piqj} = \mu_1 \delta_{ij} \delta_{pq} + \mu_2 \delta_{pj} \delta_{iq} + \lambda \delta_{ip} \delta_{jq}$, equation (4-6) can be formally written as

$$\mu_1 (\mathbf{v})_{p,ii} + (\mu_2 + \lambda) (\mathbf{v})_{q,qp} + (\mathbf{P})_{pi} (\chi_\Omega)_{,i} = 0. \quad (4-18)$$

It is easy to verify by direct calculation that \mathbf{v} defined in equation (4-17) satisfies equation (4-18) if $\mathbf{P} = \mathbf{I}$. If $\mu_2 + \lambda = 0$ then \mathbf{v} satisfying (4-17) also satisfies equation (4-18) for all $\mathbf{P} \in \mathbb{R}^{n \times n}$. This formal calculation can be made rigorous since solutions of equation (4-15) are in $W_{per}^{2,2}(Y)$.

Now we note that if Ω is a periodic E-inclusion specified by equation (2-19) with $\mathbf{Q} \in \mathbb{Q}$ (cf., (2-18)), the second equation in (2-19) and equation (4-17) imply that for any $\mathbf{P} \in \{a\mathbf{I} : a \in \mathbb{R}\}$,

$$\nabla \mathbf{v}(\mathbf{x}, \mathbf{P}) = -\frac{(1-\theta)}{\mu_1 + \mu_2 + \lambda} \mathbf{P} \mathbf{Q} \quad \text{on } \Omega \quad (4-19)$$

and

$$\mathbf{R} \mathbf{P} = \frac{\mathbf{P} \mathbf{Q}}{\mu_1 + \mu_2 + \lambda}. \quad (4-20)$$

If $\mu_2 + \lambda = 0$, equations (4-19) and (4-20) hold for all $\mathbf{P} \in \mathbb{R}^{n \times n}$ by Lemma 1. Therefore, under the conditions specified in Lemma 1, if Ω is a periodic E-inclusion then the homogeneous Eshelby problem can be used to solve the inhomogeneous Eshelby problem.

In applications to elasticity it is typically of interest to solve the inhomogeneous Eshelby inclusion problem (4-5) for given elasticity tensors \mathbf{L}_1 and \mathbf{L}_2 , as this is a model of an elastic composite. The preceding result shows that there is a periodic E-inclusion with any positive semi-definite displacement gradient on the inclusion, for \mathbf{L}_2 having the form (4-16). The volume fraction of this E-inclusion is independently assignable. The form of \mathbf{L}_2 is sufficiently general to include all isotropic elasticity tensors with the usual mild restrictions.

In applications to magnetism there are two problems of greatest interest. In ferromagnetism one usually wants to solve the magnetostatic equation $\operatorname{div}(-\nabla v + \mathbf{m}\chi_\Omega) = 0$ for given *magnetization* $\mathbf{m} \in \mathbb{R}^3$. This problem corresponds to the homogeneous Eshelby inclusion problem with $m = 1$, $n = 3$, $\mathbf{P} = \mathbf{m}$, $\mathbf{L}_2 = \mathbf{I}$. The preceding result in the case $\mu_2 = \lambda = 0$ shows that for any given $\mathbf{m} \in \mathbb{R}^3$, any periodic E-inclusion (of any volume fraction) has the property that the magnetic field $-\nabla v$ is uniform on the inclusion. Paramagnetic or diamagnetic materials are usually described by a linear relation between magnetization and magnetic field, $\mathbf{m} = \mathcal{X}(-\nabla v)$, where \mathcal{X} is the permeability tensor, and the governing equation is again $\operatorname{div}((\mathbf{I} + \mathcal{X})\nabla v) = 0$ with the average field given. A two-phase composite of such materials is described by the inhomogeneous Eshelby problem with $\mathbf{L}_{1,2} = (\mathbf{I} + \mathcal{X}_{1,2})$. The latter also describes a two-phase composite of conductive materials with $\mathbf{L}_{1,2}$ interpreted as the conductivity tensors and v as the electric potential.

We now return to the general case. From Lemma 1, equations (4-4), (4-14) and (4-19), direct calculations reveal the following explicit form for the effective tensor of a two-phase composite with one phase occupying a periodic E-inclusion.

Theorem 6. *Consider a two-phase periodic composite described by the inhomogeneous Eshelby inclusion problem (4-6) for $n = m \geq 1$, with $\mathbf{L}^e(\Omega)$ defined by (4-4) and*

$$\mathbf{L}(\mathbf{x}, \Omega) = \begin{cases} \mathbf{L}_1 \in \mathbb{L} & \mathbf{x} \in \Omega, \\ (\mathbf{L}_2)_{piqj} = \mu_1 \delta_{ij} \delta_{pq} + \mu_2 \delta_{pj} \delta_{iq} + \lambda \delta_{ip} \delta_{jq} \in \mathbb{L} & \mathbf{x} \in Y \setminus \Omega, \end{cases}$$

where Ω is a periodic E-inclusion specified by equation (2-19) with $\mathbf{Q} \in \mathbb{Q}$ given.

(i) If $\mu_2 + \lambda = 0$, then

$$\mathbf{L}^e(\Omega) = \mathbf{L}_\theta - \theta(1 - \theta) \Delta \mathbf{L} (\tilde{\mathbf{L}}_\theta + \mathbf{Y}(\mathbf{Q}))^{-1} \Delta \mathbf{L}, \quad (4-21)$$

where $\theta = |\Omega|/|Y|$, $\mathbf{L}_\theta = \theta \mathbf{L}_1 + (1 - \theta) \mathbf{L}_2$, $\tilde{\mathbf{L}}_\theta = \theta \mathbf{L}_2 + (1 - \theta) \mathbf{L}_1$, $\Delta \mathbf{L} = \mathbf{L}_2 - \mathbf{L}_1$, and the mapping $\mathbf{Y}(\mathbf{Q})$ in components is

$$(\mathbf{Y})_{piqj} = -(\mathbf{L}_2)_{piqj} + \mu_1 \delta_{pq} (\mathbf{Q}^{-1})_{ij} \quad (4-22)$$

for invertible \mathbf{Q} (see Remark 2 below).

(ii) If $\mu_2 + \lambda \neq 0$ and $\mathbf{I} \in \mathcal{R}(\Delta\mathbf{L}) = \{\text{the range of the linear mapping } \Delta\mathbf{L}\}$, then

$$\begin{aligned} \mathbf{F} \cdot \mathbf{L}^e(\Omega)\mathbf{F} &= \mathbf{F} \cdot \mathbf{L}_2\mathbf{F} \\ &+ \frac{\theta(\mu_1 + \mu_2 + \lambda)}{(1 - \theta) - (\mu_1 + \mu_2 + \lambda)\text{Tr}(\Delta\mathbf{L}^{-1}\mathbf{I})} \text{Tr}(\mathbf{F})^2 \end{aligned} \quad (4-23)$$

for all $\mathbf{F} \in \mathbb{R}^{n \times n}$ satisfying $\text{Tr}(\mathbf{F}) \neq 0$ and

$$\frac{\Delta\mathbf{L}\mathbf{F}}{\text{Tr}(\mathbf{F})} = \frac{(1 - \theta)\Delta\mathbf{L}\mathbf{Q} - (\mu_1 + \mu_2 + \lambda)\mathbf{I}}{(1 - \theta) - (\mu_1 + \mu_2 + \lambda)\text{Tr}(\Delta\mathbf{L}^{-1}\mathbf{I})}. \quad (4-24)$$

Remark 2. The meaning of the term $(\tilde{\mathbf{L}}_\theta + \mathbf{Y}(\mathbf{Q}))^{-1}$ in (4-21) in the case that \mathbf{Q} is not invertible is given by

$$(\tilde{\mathbf{L}}_\theta + \mathbf{Y}(\mathbf{Q}))^{-1} := \lim_{\varepsilon \searrow 0} (\tilde{\mathbf{L}}_\theta + \mathbf{Y}(\mathbf{Q} + \varepsilon\mathbf{I}))^{-1}. \quad (4-25)$$

Note that because of the restriction on \mathbf{F} , equation (4-23) is not sufficient to determine all components of the tensor $\mathbf{L}^e(\Omega)$. But even limited explicit results on the effective tensor are rare in the theory of composites.

Proof. Let us first assume that $\mu_2 + \lambda = 0$ and that Ω is a periodic E-inclusion corresponding to \mathbf{Q} (cf., (2-18)). MILTON ([43], page 397) has shown that the effective tensor can be equivalently written as equation (4-21) in terms of “ \mathbf{Y} -tensor”, which satisfies

$$\begin{aligned} \mathbf{Y} \left(\int_{\Omega} \nabla \mathbf{v} d\mathbf{x} \right) &= - \int_{\Omega} \{ \mathbf{L}_1(\nabla \mathbf{v} + \mathbf{F}) \\ &- \int_{\mathbf{Y}} [\mathbf{L}(\mathbf{x}, \Omega)(\nabla \mathbf{v} + \mathbf{F})] d\mathbf{x} \} d\mathbf{y}. \end{aligned} \quad (4-26)$$

From equations (4-12), (4-19) and (4-26), direct calculations show that \mathbf{Y} is given by (4-22) in the case that \mathbf{Q} is invertible. If \mathbf{Q} is not invertible, then one still recovers equation (4-21) with the definition given in Remark 2.

If $\mu_2 + \lambda \neq 0$, Lemma 1 implies equation (4-7) holds for all $\mathbf{P} = a\mathbf{I}$ ($0 \neq a \in \mathbb{R}$) and therefore equation (4-14) is valid for all \mathbf{F} that satisfy equation (4-12). Since $\mathbf{I} \in \mathcal{R}(\Delta\mathbf{L})$, equations (4-19) and (4-12) imply that

$$(\mu_1 + \mu_2 + \lambda)\text{Tr}(\mathbf{F}) = a[(1 - \theta) - (\mu_1 + \mu_2 + \lambda)\text{Tr}(\Delta\mathbf{L}^{-1}\mathbf{I})],$$

and hence equation (4-12) can be rewritten as equation (4-24). Also,

$$\begin{aligned} \mathbf{F} \cdot \mathbf{P} &= a\mathbf{F} \cdot \mathbf{I} = a\text{Tr}(\mathbf{F}) \\ &= \frac{(\mu_1 + \mu_2 + \lambda)\text{Tr}(\mathbf{F})^2}{(1 - \theta) - (\mu_1 + \mu_2 + \lambda)\text{Tr}(\Delta\mathbf{L}^{-1}\mathbf{I})}, \end{aligned} \quad (4-27)$$

which, by equation (4-14), implies equation (4-23).

Remark 3. The special form of \mathbf{L}_2 has played an important role in connecting the scalar problem (4-15) and the vector problem (4-6). The restriction on \mathbf{L}_2 in Lemma 1 and Theorem 6 can be relaxed to satisfy the weaker restriction

$$(\mathbf{L}_2)_{piqj}(\hat{\mathbf{k}})_i(\hat{\mathbf{k}})_j(\hat{\mathbf{k}})_q = \kappa(\hat{\mathbf{k}})_p \quad \forall |\hat{\mathbf{k}}| = 1 \quad \text{and} \quad \mathbf{L}_2 \in \mathbb{L}, \quad (4-28)$$

where $\kappa > 0$ is a constant. To show this, one notices that, by Fourier expansion (KHACHATURYAN [29]; MURA [45]), the gradient of the solution of equation (4-6) can be represented as

$$[\nabla \mathbf{v}]_{pi} = \sum_{\mathbf{k} \in \mathcal{K} \setminus \{0\}} \frac{-1}{(2\pi)^n} \hat{\chi}_\Omega(\mathbf{k}) N_{pq}(\hat{\mathbf{k}}) (\hat{\mathbf{k}})_i (\hat{\mathbf{k}})_j (\mathbf{P})_{jq} \exp(i\mathbf{k} \cdot \mathbf{x}), \quad (4-29)$$

where \mathcal{K} is the reciprocal lattice of lattice \mathcal{L} , $\hat{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$, $N_{pq}(\hat{\mathbf{k}})$ is the inverse of the matrix $(\mathbf{L}_2)_{piqj}(\hat{\mathbf{k}})_i(\hat{\mathbf{k}})_j$, and $\hat{\chi}_\Omega(\mathbf{k})$ is the Fourier transformation of $\chi_\Omega(\mathbf{x})$

$$\hat{\chi}_\Omega(\mathbf{k}) = \int_{\mathbf{Y}} \chi_\Omega(\mathbf{x}) \exp(-i\mathbf{k} \cdot \mathbf{x}) d\mathbf{x}.$$

Therefore, the linear mapping \mathbf{R} of (4-8) can always be represented as

$$\begin{aligned} (\mathbf{R})_{piqj} &= \sum_{\mathbf{k} \in \mathcal{K} \setminus \{0\}} \frac{1}{\theta(1-\theta)(2\pi)^n} N_{pq}(\hat{\mathbf{k}}) (\hat{\mathbf{k}})_i (\hat{\mathbf{k}})_j \\ &\quad \int_{\Omega} \int_{\Omega} \exp(i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')) d\mathbf{x}' d\mathbf{x}. \end{aligned} \quad (4-30)$$

Similarly, the second gradient of the solution of problem (4-15) can be represented as

$$[\nabla \nabla u(\mathbf{x})]_{pi} = \sum_{\mathbf{k} \in \mathcal{K} \setminus \{0\}} \frac{-1}{(2\pi)^n} \hat{\chi}_\Omega(\mathbf{k}) (\hat{\mathbf{k}})_i (\hat{\mathbf{k}})_p \exp(i\mathbf{k} \cdot \mathbf{x}). \quad (4-31)$$

By comparing (4-29) with (4-31), we note that that if equation (4-28) holds, i.e.,

$$N_{pq}(\hat{\mathbf{k}}) (\hat{\mathbf{k}})_q = \frac{1}{\kappa} (\hat{\mathbf{k}})_p \quad \forall |\hat{\mathbf{k}}| = 1,$$

then for $\mathbf{P} = \mathbf{I}$,

$$\nabla \mathbf{v} = \frac{\nabla \nabla u(\mathbf{x})}{\kappa}. \quad (4-32)$$

This shows that under the weaker restriction (4-16) on \mathbf{L}_2 , the scalar problem (4-15) generates a solution of homogeneous Eshelby inclusion problem (4-6).

Remark 4. It is useful to notice that if \mathbf{L}_2 satisfies (4-28), the energy of the homogeneous Eshelby inclusion problem (4-6) for $\mathbf{P} = \mathbf{I}$ depends only on the volume fraction of Ω . To see this, we notice by equations (4-8) and (4-32),

$$\mathbf{I} \cdot \mathbf{R}\mathbf{I} = \frac{-1}{(1-\theta)\kappa} \mathbf{I} \cdot \left[\int_{\Omega} \nabla \nabla u d\mathbf{x} \right] = \frac{-1}{\kappa\theta(1-\theta)} \int_Y \chi_{\Omega} \Delta u d\mathbf{x} = \frac{1}{\kappa}, \quad (4-33)$$

which, together with (4-9), implies

$$\int_Y \nabla \mathbf{v}(\mathbf{x}, \mathbf{I}) \cdot \mathbf{L}_2 \nabla \mathbf{v}(\mathbf{x}, \mathbf{I}) d\mathbf{x} = \frac{\theta(1-\theta)}{\kappa}. \quad (4-34)$$

In the context of linearized elasticity, equation (4-34) is referred to as the Bitter-Crum theorem (BITTER [5]; CRUM [9]; CAHN & LARCHE [7]). Also, from the positive semi-definiteness of $\mathbf{R}\mathbf{I}$ (cf., (4-30)) we have

$$\mathbf{R}\mathbf{I} = \frac{1}{\kappa} \mathbf{Q} \quad (4-35)$$

for some $\mathbf{Q} \in \mathbb{Q}$ (cf., (2-18)).

4.2. Periodic E-inclusions as energy-minimizing structures for two-phase composites

In this section, we consider the minimization/maximization problems over measurable Ω with fixed volume fraction θ (cf., equation (4-3))

$$J_{\theta}^l(\mathbf{F}) = \inf_{|\Omega|/|Y|=\theta} \{ J_*(\mathbf{L}, \mathbf{F}, \Omega) = \frac{1}{2} \mathbf{F} \cdot \mathbf{L}^e(\Omega) \mathbf{F} \} \quad (4-36)$$

and

$$J_{\theta}^u(\mathbf{F}) = \sup_{|\Omega|/|Y|=\theta} \{ J_*(\mathbf{L}, \mathbf{F}, \Omega) = \frac{1}{2} \mathbf{F} \cdot \mathbf{L}^e(\Omega) \mathbf{F} \}. \quad (4-37)$$

If the infimum (resp. supremum) of problem (4-36) (resp. (4-37)) is attained by Ω_* (resp. Ω^*)

$$\frac{1}{2} \mathbf{F} \cdot \mathbf{L}^e(\Omega_*) \mathbf{F} = J_{\theta}^l(\mathbf{F}) \quad (\text{resp.} \quad \frac{1}{2} \mathbf{F} \cdot \mathbf{L}^e(\Omega^*) \mathbf{F} = J_{\theta}^u(\mathbf{F})),$$

then the region Ω_* (resp. Ω^*), corresponding to the optimal composite of least (resp. greatest) moduli, is referred to as *an energy-minimizing structure*³. Below we will show that periodic E-inclusions are energy-minimizing for $J_*(\mathbf{L}, \mathbf{F}, \Omega)$ under suitable hypotheses on the tensors \mathbf{L}_1 and \mathbf{L}_2 .

The energy $J_*(\mathbf{L}, \mathbf{F}, \Omega)$, as a function of Ω , is not amenable to the direct method of the calculus of variations. We turn to an indirect method

³ If $J_*(\mathbf{L}, \mathbf{F}, \Omega^*) = J_{\theta}^u(\mathbf{F})$, from the duality of convex functions, Ω^* minimizes the corresponding complementary energy $\hat{J}_*(\mathbf{L}, \mathbf{P}, \Omega) := \sup\{\mathbf{F} \cdot \mathbf{P} - J_*(\mathbf{L}, \mathbf{F}, \Omega) : \mathbf{F} \in \mathbb{R}^{m \times n}\}$.

which is by now standard. The idea is that, one first finds a structure-independent bound, and then studies if the bound can be attained and, if so, by what kind of structures. Among many methods of deriving bounds on the effective properties of composites, the Hashin-Shtrikman variational method (HASHIN & SHTRIKMAN [22, 23]) and the method of compensated compactness (TARTAR [50]) or translation (LURIE & CHERKAEV [39]) have proven to be useful in many situations. For a comprehensive treatment of these methods, readers are referred to MILTON [43].

For the moment, in addition to self-adjointness, we assume \mathbf{L}_1 and \mathbf{L}_2 are *positive definite*. To be able to relate the homogeneous Eshelby inclusion problem (4-6) with the scalar problem (4-15), we again assume that $m = n \geq 1$ and $(\mathbf{L}_2)_{piqj} = \mu_1 \delta_{ij} \delta_{pq} + \mu_2 \delta_{pj} \delta_{iq} + \lambda \delta_{ip} \delta_{jq}$, where $\mu_1 > \mu_2$, $\mu_1 + \mu_2 > 0$ and $\lambda > -(\mu_1 + \mu_2)/n$. The restriction of \mathbf{L}_1 and \mathbf{L}_2 being positive definite can be replaced by the weaker one that $\mathbf{L}_1 \in \mathbb{L}$ and $\mathbf{L}_2 \in \mathbb{L}$, see Remark 5.

For a two-phase composite (4-1), let us recall $\mathbf{L}^e(\Omega)$ is defined by (4-4). The lower and upper Hashin-Shtrikman variational principles (MILTON & KOHN [44]) are

(i) If $\mathbf{L}_1 \geq \mathbf{L}_2 > 0$ and $t \in (0, 1)$,

$$\begin{aligned} \mathbf{P} \cdot (\mathbf{L}^e(\Omega) - t\mathbf{L}_2)^{-1} \mathbf{P} = \min_{\mathbf{B} \in \mathcal{B}(\mathbf{P})} \left\{ \int_Y [\nabla \mathbf{v}_\mathbf{B} \cdot t\mathbf{L}_2 \nabla \mathbf{v}_\mathbf{B} \right. & \quad (4-38) \\ \left. + \mathbf{B}(\mathbf{x}) \cdot (\mathbf{L}(\mathbf{x}, \Omega) - t\mathbf{L}_2)^{-1} \mathbf{B}(\mathbf{x})] d\mathbf{x} \right\}, \end{aligned}$$

(ii) If $0 < \mathbf{L}_1 \leq \mathbf{L}_2$ and $t > 1$,

$$\begin{aligned} \mathbf{P} \cdot (t\mathbf{L}_2 - \mathbf{L}^e(\Omega))^{-1} \mathbf{P} = \min_{\mathbf{B} \in \mathcal{B}(\mathbf{P})} \left\{ \int_Y [-\nabla \mathbf{v}_\mathbf{B} \cdot t\mathbf{L}_2 \nabla \mathbf{v}_\mathbf{B} \right. & \quad (4-39) \\ \left. + \mathbf{B}(\mathbf{x}) \cdot (t\mathbf{L}_2 - \mathbf{L}(\mathbf{x}, \Omega))^{-1} \mathbf{B}(\mathbf{x})] d\mathbf{x} \right\}. \end{aligned}$$

The inclusion of the scalar t ensures that inverses are well-defined in the context of $\mathbf{L}_2 \leq \mathbf{L}^e(\Omega) \leq \mathbf{L}_1$ (resp., $\mathbf{L}_1 \leq \mathbf{L}^e(\Omega) \leq \mathbf{L}_2$). In both equations (4-38) and (4-39),

$$\mathcal{B}(\mathbf{P}) := \{\mathbf{B}(\mathbf{x}) \in L^2(Y, \mathbb{R}^{n \times n}) : \int_Y \mathbf{B}(\mathbf{x}) d\mathbf{x} = \mathbf{P}\},$$

and $\mathbf{v}_\mathbf{B} \in W_{per}^{1,2}(Y; \mathbb{R}^n)$ satisfies

$$\begin{cases} \operatorname{div}[t\mathbf{L}_2 \nabla \mathbf{v}_\mathbf{B} + \mathbf{B}(\mathbf{x})] = 0 & \text{on } Y, \\ \text{periodic boundary conditions} & \text{on } \partial Y. \end{cases} \quad (4-40)$$

In the terminology of Hashin and Shtrikman, we are using $t\mathbf{L}_2$ as the *comparison material*. For any $\mathbf{P} \in \mathbb{R}^{n \times n}$, choose $\mathbf{B}(\mathbf{x}) = \frac{1}{\theta} \mathbf{P} \chi_\Omega(\mathbf{x})$ in (4-38), (4-39). Then, using (4-9), it follows that

(i) if $0 < \mathbf{L}_2 \leq \mathbf{L}_1$, $t \in (0, 1)$,

$$0 < (\mathbf{L}^e(\Omega) - t\mathbf{L}_2)^{-1} \leq \left[\frac{1-\theta}{\theta t} \mathbf{R} + \frac{1}{\theta} (\mathbf{L}_1 - t\mathbf{L}_2)^{-1} \right], \quad (4-41)$$

(ii) if $0 < \mathbf{L}_1 \leq \mathbf{L}_2$, $t > 1$,

$$0 < (t\mathbf{L}_2 - \mathbf{L}^e(\Omega))^{-1} \leq \left[-\frac{1-\theta}{\theta t} \mathbf{R} - \frac{1}{\theta} (\mathbf{L}_1 - t\mathbf{L}_2)^{-1} \right]. \quad (4-42)$$

Note that, in equations (4-41) and (4-42), the tensor \mathbf{R} is defined by equation (4-8), and hence by equation (4-33),

$$\mathbf{I} \cdot \mathbf{R} \mathbf{I} = \frac{1}{(\mu_1 + \mu_2 + \lambda)}. \quad (4-43)$$

To evaluate the bounds (4-41) and (4-42), the operation $\mathbf{I} \cdot (\) \mathbf{I}$ is applied to both sides of (4-41) and (4-42). If $\mathbf{I} \in \mathcal{R}(\Delta \mathbf{L}) = \{\text{the range of } \Delta \mathbf{L} = \mathbf{L}_2 - \mathbf{L}_1\}$, from equation (4-43) we know the left-hand sides of (4-41) and (4-42) are bounded as $t \rightarrow 1$, which implies $\mathbf{I} \in \mathcal{R}(\mathbf{L}^e(\Omega) - \mathbf{L}_2)$. If the inverse is understood as being restricted to $\mathcal{R}(\mathbf{L}^e(\Omega) - \mathbf{L}_2)$, sending $t \rightarrow 1$ we obtain the following structure-independent Hashin-Shtrikman bounds:

(i) if $0 < \mathbf{L}_2 \leq \mathbf{L}_1$,

$$\mathbf{I} \cdot (\mathbf{L}^e(\Omega) - \mathbf{L}_2)^{-1} \mathbf{I} \leq \frac{1-\theta}{\theta(\mu_1 + \mu_2 + \lambda)} - \frac{1}{\theta} \mathbf{I} \cdot \Delta \mathbf{L}^{-1} \mathbf{I}, \quad (4-44)$$

(ii) if $0 < \mathbf{L}_1 \leq \mathbf{L}_2$,

$$\mathbf{I} \cdot (\mathbf{L}_2 - \mathbf{L}^e(\Omega))^{-1} \mathbf{I} \leq -\frac{1-\theta}{\theta(\mu_1 + \mu_2 + \lambda)} + \frac{1}{\theta} \mathbf{I} \cdot \Delta \mathbf{L}^{-1} \mathbf{I}. \quad (4-45)$$

Note that $0 < \mathbf{L}_2 \leq \mathbf{L}_1$ implies $\mathbf{L}^e(\Omega) - \mathbf{L}_2 \geq 0$. From the duality of convex functions, the first inequality in (4-44) can be rewritten as

$$\begin{aligned} \sup_{\mathbf{F} \in \mathbb{R}^{n \times n}} \{2\mathbf{I} \cdot \mathbf{F} - \mathbf{F} \cdot (\mathbf{L}^e(\Omega) - \mathbf{L}_2) \mathbf{F}\} &= \mathbf{I} \cdot (\mathbf{L}^e(\Omega) - \mathbf{L}_2)^{-1} \mathbf{I} \quad (4-46) \\ &\leq \frac{1-\theta}{\theta(\mu_1 + \mu_2 + \lambda)} - \frac{1}{\theta} \mathbf{I} \cdot \Delta \mathbf{L}^{-1} \mathbf{I} =: c_*. \end{aligned}$$

Clearly, $c_* \neq 0$ since $\mathbf{I} \in \mathcal{R}(\mathbf{L}^e(\Omega) - \mathbf{L}_2)$ for any Ω with $|\Omega|/|Y| = \theta$. Choosing \mathbf{F} with $\text{Tr}(\mathbf{F}) = c_*$, we have $2c_* - \mathbf{F} \cdot (\mathbf{L}^e(\Omega) - \mathbf{L}_2) \mathbf{F} \leq c_*$, and hence

$$\begin{aligned} \mathbf{F} \cdot (\mathbf{L}^e(\Omega) - \mathbf{L}_2) \mathbf{F} &\geq c_* = \text{Tr}(\mathbf{F})^2 / c_* \quad (4-47) \\ &= \frac{\theta(\mu_1 + \mu_2 + \lambda)}{(1-\theta) - (\mu_1 + \mu_2 + \lambda) \text{Tr}(\Delta \mathbf{L}^{-1} \mathbf{I})} \text{Tr}(\mathbf{F})^2. \end{aligned}$$

For any $\mathbf{F} \in \mathbb{R}^{n \times n}$, if $\text{Tr}(\mathbf{F}) = 0$, the above inequality clearly holds. If $\text{Tr}(\mathbf{F}) \neq 0$, we apply the inequality to $c_* \mathbf{F} / \text{Tr}(\mathbf{F})$. Thus, we conclude that

the inequality (4-47) holds for any $\mathbf{F} \in \mathbb{R}^{n \times n}$. By a similar argument applied to the second inequality in (4-45), we conclude that if $0 < \mathbf{L}_1 \leq \mathbf{L}_2$ and $\mathbf{I} \in \mathcal{R}(\Delta \mathbf{L})$,

$$\mathbf{F} \cdot (\mathbf{L}^e(\Omega) - \mathbf{L}_2)\mathbf{F} \leq \frac{\theta(\mu_1 + \mu_2 + \lambda)}{(1 - \theta) - (\mu_1 + \mu_2 + \lambda)\text{Tr}(\Delta \mathbf{L}^{-1}\mathbf{I})} \text{Tr}(\mathbf{F})^2. \quad (4-48)$$

for any $\mathbf{F} \in \mathbb{R}^{n \times n}$.

From Theorem 6, equations (4-47) and (4-48), we have

Theorem 7. *Consider a periodic composite defined by*

$$\mathbf{L}(\mathbf{x}, \Omega) = \begin{cases} \mathbf{L}_1 & \mathbf{x} \in \Omega, \\ (\mathbf{L}_2)_{piqj} = \mu_1 \delta_{ij} \delta_{pq} + \mu_2 \delta_{pj} \delta_{iq} + \lambda \delta_{ip} \delta_{jq} & \mathbf{x} \in Y \setminus \Omega, \end{cases} \quad (4-49)$$

where $\mathbf{L}_1, \mathbf{L}_2$ are self-adjoint and positive definite and $\mathbf{I} \in \mathcal{R}(\Delta \mathbf{L})$.

(i) If $\mathbf{L}_1 \geq \mathbf{L}_2$, then for any $|\Omega|/|Y| = \theta$ and any $\mathbf{F} \in \mathbb{R}^{n \times n}$,

$$\begin{aligned} & \mathbf{F} \cdot \mathbf{L}^e(\Omega)\mathbf{F} - \mathbf{F} \cdot \mathbf{L}_2\mathbf{F} \\ & \geq \frac{\theta(\mu_1 + \mu_2 + \lambda)}{(1 - \theta) - (\mu_1 + \mu_2 + \lambda)\text{Tr}(\Delta \mathbf{L}^{-1}\mathbf{I})} \text{Tr}(\mathbf{F})^2. \end{aligned} \quad (4-50)$$

Further, if $\mathbf{Q} \in \mathbb{Q}$ and \mathbf{F} with $\text{Tr}(\mathbf{F}) \neq 0$ satisfy

$$\frac{\Delta \mathbf{L}\mathbf{F}}{\text{Tr}(\mathbf{F})} = \frac{(1 - \theta)\Delta \mathbf{L}\mathbf{Q} - (\mu_1 + \mu_2 + \lambda)\mathbf{I}}{(1 - \theta) - (\mu_1 + \mu_2 + \lambda)\text{Tr}(\Delta \mathbf{L}^{-1}\mathbf{I})}, \quad (4-51)$$

then inequality (4-50) holds as an equality with Ω being a periodic E-inclusion corresponding to \mathbf{Q} and volume fraction θ .

(ii) If $\mathbf{L}_1 \leq \mathbf{L}_2$, then for any $|\Omega|/|Y| = \theta$ and any $\mathbf{F} \in \mathbb{R}^{n \times n}$,

$$\begin{aligned} & \mathbf{F} \cdot \mathbf{L}^e(\Omega)\mathbf{F} - \mathbf{F} \cdot \mathbf{L}_2\mathbf{F} \\ & \leq \frac{\theta(\mu_1 + \mu_2 + \lambda)}{(1 - \theta) - (\mu_1 + \mu_2 + \lambda)\text{Tr}(\Delta \mathbf{L}^{-1}\mathbf{I})} \text{Tr}(\mathbf{F})^2. \end{aligned} \quad (4-52)$$

Further, if $\mathbf{Q} \in \mathbb{Q}$ and \mathbf{F} with $\text{Tr}(\mathbf{F}) \neq 0$ satisfy equation (4-51), then inequality (4-52) holds as an equality with Ω being a periodic E-inclusion corresponding to \mathbf{Q} and volume fraction θ .

Remark 5. For Theorem 7, the restriction of $\mathbf{L}_{1,2}$ being positive definite can be replaced by $\mathbf{L}_{1,2} \in \mathbb{L}$ (cf. (4-2)). To see this, let us consider equation (4-3). By replacing $\mathbf{L}(\mathbf{x}, \Omega)$ by $\mathbf{L}_\varepsilon(\mathbf{x}, \Omega) = \mathbf{L}(\mathbf{x}, \Omega) + \varepsilon \mathbf{II}$ ($\varepsilon \in [0, 1]$, $(\mathbf{II})_{piqj} = \delta_{ij} \delta_{pq}$), we define $\mathbf{L}_\varepsilon^e(\Omega)$ as for any $\mathbf{F} \in \mathbb{R}^{n \times n}$,

$$\mathbf{F} \cdot \mathbf{L}_\varepsilon^e(\Omega)\mathbf{F} = \min_{\mathbf{v} \in W_{per}^{1,2}(Y; \mathbb{R}^n)} \int_Y (\nabla \mathbf{v} + \mathbf{F}) \cdot \mathbf{L}_\varepsilon(\mathbf{x}, \Omega)(\nabla \mathbf{v} + \mathbf{F}) d\mathbf{x}. \quad (4-53)$$

We now show

$$\lim_{\varepsilon \rightarrow 0} \mathbf{F} \cdot \mathbf{L}_\varepsilon^e(\Omega) \mathbf{F} = \mathbf{F} \cdot \mathbf{L}^e(\Omega) \mathbf{F} \quad \forall \mathbf{F} \in \mathbb{R}^{n \times n}. \quad (4-54)$$

It is clear that it is sufficient to prove (4-54) for all \mathbf{F} with $|\mathbf{F}| = 1$. Let $\mathbf{v}_\mathbf{F}$ be a minimizer of (4-53) with $\varepsilon = 0$ and $|\mathbf{F}| = 1$. Since $\mathbf{L}_{1,2}$ belong to \mathbb{L} , using Korn's inequality (DUVAUT & LIONS [11]) if necessary, we know there exists $M > 0$, independent of $\mathbf{F} \in \{|\mathbf{F}| = 1\}$, such that

$$\int_Y |\nabla \mathbf{v}_\mathbf{F} + \mathbf{F}|^2 d\mathbf{x} \leq M. \quad (4-55)$$

Choosing $\mathbf{v} = \mathbf{v}_\mathbf{F}$ in (4-53) for any $\varepsilon > 0$, we have

$$\mathbf{F} \cdot \mathbf{L}^e(\Omega) \mathbf{F} \leq \mathbf{F} \cdot \mathbf{L}_\varepsilon^e(\Omega) \mathbf{F} \leq \mathbf{F} \cdot \mathbf{L}^e(\Omega) \mathbf{F} + \varepsilon \left[\int_Y |\nabla \mathbf{v}_\mathbf{F} + \mathbf{F}|^2 d\mathbf{x} \right], \quad (4-56)$$

where the first inequality follows directly from $\mathbf{L}_\varepsilon(\mathbf{x}, \Omega) > \mathbf{L}(\mathbf{x}, \Omega)$. From equations (4-55)-(4-56) we obtain equation (4-54) by sending $\varepsilon \rightarrow 0$.

Therefore, if $\mathbf{L}_{1,2} \in \mathbb{L}$, Theorem 7 applied to $\mathbf{L}_\varepsilon(\mathbf{x}, \Omega) = \mathbf{L}(\mathbf{x}, \Omega) + \varepsilon \mathbf{I}$ imply that if $\mathbf{I} \in \mathcal{R}(\Delta \mathbf{L})$, $\mathbf{L}_1 \geq \mathbf{L}_2$ and $|\Omega| = \theta$, then equation (4-50) reads

$$\begin{aligned} \mathbf{F} \cdot \mathbf{L}_\varepsilon^e(\Omega) \mathbf{F} &\geq \mathbf{F} \cdot \mathbf{L}_2 \mathbf{F} + \varepsilon |\mathbf{F}|^2 \\ &+ \frac{\theta(\mu_1 + \mu_2 + \lambda + \varepsilon)}{(1 - \theta) - (\mu_1 + \mu_2 + \lambda + \varepsilon) \text{Tr}(\Delta \mathbf{L}^{-1} \mathbf{I})} \text{Tr}(\mathbf{F})^2 \quad \forall \mathbf{F} \in \mathbb{R}^{n \times n}. \end{aligned} \quad (4-57)$$

Also, equation (4-51) becomes

$$\frac{\Delta \mathbf{L} \mathbf{F}}{\text{Tr}(\mathbf{F})} = \frac{(1 - \theta) \Delta \mathbf{L} \mathbf{Q} - (\mu_1 + \mu_2 + \lambda + \varepsilon) \mathbf{I}}{(1 - \theta) - (\mu_1 + \mu_2 + \lambda + \varepsilon) \text{Tr}(\Delta \mathbf{L}^{-1} \mathbf{I})}. \quad (4-58)$$

Sending $\varepsilon \rightarrow 0$ and making use of equation (4-54) and the continuity of the right-hand sides of (4-57) and (4-58), we conclude that part (i) of Theorem 7 remains valid with the assumption that $\mathbf{L}_{1,2} \in \mathbb{L}$ in place of $\mathbf{L}_{1,2}$ being positive definite. The upper bound (4-52) is handled similarly.

Remark 6. It is well-known that there exist many structures that achieve the optimal bounds (4-44) and (4-45) or (4-50) and (4-52). For instance, coated spheres, confocal ellipsoids, multicoated spheres multi-rank laminations, and Sigmund's constructions can achieve the optimal bounds (4-50) and (4-52) in various cases, see HASHIN & SHTRIKMAN [21, 23]; MILTON [42]; LURIE & CHERKAEV [40]; ALLAIRE & KOHN [1, 2, 3]; GRABOVSKY & KOHN [19, 20]; SIGMUND [49] and GIBIANSKY & SIGMUND [16]. All these constructions in general involve the assembly of some fundamental structures at different length scales. In mathematical terminology, they are minimizing sequences instead of minimizers. Quite differently, periodic E-inclusions are indeed minimizers for energy function $J_*(\mathbf{L}, \mathbf{F}, \Omega)$. Moreover, if restricted to periodic structures and assuming $\mathcal{R}(\Delta \mathbf{L}) \supset \mathbb{R}_{sym}^{n \times n}$, we can

show that the structures attaining the optimal bounds (4-50) or (4-52) must be the periodic E-inclusions specified by equation (2-19) (LIU [35]).

Remark 7. If we apply linear transformations

$$\mathbf{x} \longrightarrow \mathbf{x}' = \Lambda^{-1}\mathbf{x} \quad \text{and} \quad \mathbf{v} \longrightarrow \mathbf{v}' = \mathbf{G}^{-1}\mathbf{v}, \quad (4-59)$$

to equation (4-5), we can generalize Theorems 6 and 7 with \mathbf{L}_2 of form

$$(\mathbf{L}_2)_{piqj} = \mu_1(\mathbf{G}^T \mathbf{G})_{pq}(\Lambda \Lambda^T)_{ij} + \mu_2(\mathbf{G}^T \Lambda^T)_{pj}(\mathbf{G}^T \Lambda^T)_{qi} \\ + \lambda(\mathbf{G}^T \Lambda^T)_{pi}(\mathbf{G}^T \Lambda^T)_{qj},$$

where $\mathbf{G}, \Lambda \in \mathbb{R}^{n \times n}$ are any nonsingular matrices. These changes of variables give inclusions with constant field, but, in some cases, the inclusions are not strictly E-inclusions. These changes of variables can be used to change the periodicity and the values of the field $\nabla \mathbf{v}$ on the inclusion.

Remark 8. From Remark 3 one can generalize Theorems 6 and 7 to the case of \mathbf{L}_2 satisfying equation (4-28). The linear transformations (4-59) can be applied to these \mathbf{L}_2 to further generalize Theorems 6 and 7.

Remark 9. Consider two isotropic elasticity tensors $(\mathbf{L}_2)_{piqj} = \mu_2 \delta_{ij} \delta_{pq} + \mu_2 \delta_{pj} \delta_{iq} + \lambda_2 \delta_{ip} \delta_{jq}$ and $(\mathbf{L}_1)_{piqj} = \mu_1 \delta_{ij} \delta_{pq} + \mu_1 \delta_{pj} \delta_{iq} + \lambda_1 \delta_{ip} \delta_{jq}$ with Lamé moduli $\mu_2 \leq \mu_1$ and $\lambda_2 < \lambda_1$. The volume fraction of material \mathbf{L}_1 is fixed at θ and we denote by \mathbf{L}_θ^e the effective elasticity tensor of the composite. Equations (4-50) and (4-52) imply that for any $\mathbf{F} \in \mathbb{R}_{sym}^{n \times n}$,

$$\mathbf{F} \cdot \mathbf{L}_2 \mathbf{F} + \theta \left[\frac{(2\mu_2 + \lambda_2) \text{Tr}(\mathbf{F})^2}{(1 - \theta) - \varrho} \right] \leq \mathbf{F} \cdot \mathbf{L}_\theta^e \mathbf{F} \quad (4-60) \\ \leq \mathbf{F} \cdot \mathbf{L}_1 \mathbf{F} + (1 - \theta) \left[\frac{(2\mu_1 + \lambda_1) \text{Tr}(\mathbf{F})^2}{\theta + \varrho'} \right],$$

where $\varrho = \frac{n(2\mu_2 + \lambda_2)}{2(\mu_2 - \mu_1) + n(\lambda_2 - \lambda_1)}$ and $\varrho' = \frac{2\mu_1 + \lambda_1}{2\mu_2 + \lambda_2} \varrho$. Further, the lower bound is sharp for all \mathbf{F} satisfying $\text{Tr}(\mathbf{F}) \neq 0$ and

$$a \Delta \mathbf{L} \mathbf{F} = (1 - \theta) \Delta \mathbf{L} \mathbf{Q} - (2\mu_2 + \lambda_2) \mathbf{I} \quad (4-61)$$

for some $\mathbf{Q} \in \mathbb{Q}$ and $0 \neq a \in \mathbb{R}$. Also, the upper bound is sharp for all \mathbf{F} satisfying $\text{Tr}(\mathbf{F}) \neq 0$ and

$$a \Delta \mathbf{L} \mathbf{F} = \theta \Delta \mathbf{L} \mathbf{Q} + (2\mu_1 + \lambda_1) \mathbf{I} \quad (4-62)$$

for some $\mathbf{Q} \in \mathbb{Q}$ and $0 \neq a \in \mathbb{R}$. These bounds (4-60) have been previously derived by WALPOLE [54]. In two dimensions and subjected to similar restrictions as (4-61) and (4-62), the bounds (4-60) has been proved to be attainable by ‘‘Vigdergauz structures’’, or ‘‘periodic E-inclusions’’ in our terminology, and by confocal ellipses, see GRABOVSKY & KOHN [19, 20].

Remark 10. Consider two-phase composites with conductivity tensors $0 < \mathbf{A}_1, \mathbf{A}_2 \in \mathbb{R}_{sym}^{n \times n}$ and $\Delta \mathbf{A} = \mathbf{A}_2 - \mathbf{A}_1 < 0$. We can adapt Theorems 6 and 7

by setting $(\mathbf{L}_2)_{piqj} = \delta_{pq}(\mathbf{A}_2)_{ij}$ and $(\mathbf{L}_1)_{piqj} = \delta_{pq}(\mathbf{A}_1)_{ij}$. After appropriate linear transformations (cf., Remark 7) and some algebraic calculations, from equations (4-44) and (4-45) we obtain

$$\begin{aligned}\mathrm{Tr}(\mathbf{A}_2(\mathbf{A}^e(\Omega) - \mathbf{A}_2)^{-1}) &\leq \frac{1}{\theta}\mathrm{Tr}(\mathbf{A}_2(\mathbf{A}_1 - \mathbf{A}_2)^{-1}) + \frac{1-\theta}{\theta}, \\ \mathrm{Tr}(\mathbf{A}_1(\mathbf{A}_1 - \mathbf{A}^e(\Omega))^{-1}) &\leq \frac{1}{1-\theta}\mathrm{Tr}(\mathbf{A}_1(\mathbf{A}_1 - \mathbf{A}_2)^{-1}) - \frac{\theta}{1-\theta}.\end{aligned}$$

These bounds, called the ‘‘trace bounds’’ in the literature, have been previously obtained by MILTON & KOHN [44] and have been proved to be attainable by GRABOVSKY [18].

5. Summary and discussion

We have shown the existence of special inclusions for which the overdetermined problems (1-4)-(1-5) and (1-6)-(1-7) admit a solution. They are constructed as the coincident set of a simple variational inequality with respect to piecewise quadratic obstacles. These structures are called *E-inclusions* based on their analogy with ellipsoids and their extremal properties for energy minimization problems in homogenization theory. Important restrictions on the parameters which characterize a periodic E-inclusion, namely, the matrices \mathbb{K} and volume fractions Θ , have also been derived, see equation (2-16). Numerical studies have revealed the diversity of periodic E-inclusions. The same situation is expected for nonperiodic E-inclusions.

It is of interest in the above to know what are the restrictions on the symmetric matrices $\mathbb{K} = (\mathbf{Q}_1, \dots, \mathbf{Q}_N)$ and volume fractions $\Theta = (\theta_1, \dots, \theta_N)$ for which we can find periodic E-inclusions. Let $u \in W_{per}^{2,2}(Y)$ be a solution of (1-6) associated to a periodic E-inclusion. Using L^p estimates for the Laplace operator we see that u is in fact bounded in $W_{per}^{2,p}(Y)$ for any $1 \leq p < \infty$ since Δu is bounded in $L_{per}^\infty(Y)$ (GILBARG & TRUDINGER [17], page 235). Then we can rescale it and get a sequence $u^{(k)}(\mathbf{x}) = (1/k^2)u(k\mathbf{x})\chi_D(\mathbf{x})$ for an open bounded domain D . The corresponding sequence of gradients $\mathbf{v}^{(k)}(\mathbf{x}) = \nabla u^{(k)}(\mathbf{x}) = (1/k)\nabla u(k\mathbf{x})$ is bounded in $W^{1,p}(D, \mathbb{R}^n)$ for any $1 \leq p < \infty$. The study of the gradient Young measure of the sequence $\mathbf{v}^{(k)}$ gives natural restrictions on \mathbb{K} and volume fractions Θ . For this and other purposes it is useful to define the concept of a sequential E-inclusion. A **sequential E-inclusion** is a homogeneous gradient Young measure that is generated by a sequence bounded in $W^{1,p}(D)$ for any $1 \leq p < \infty$, has zero center of mass, and satisfies

$$\nu = \sum_{i=1}^N \theta_i \delta_{\mathbf{Q}_i} + \theta_0 \mu, \quad (5-1)$$

where $\theta_1, \dots, \theta_N \geq 0$, $\theta_0 = 1 - \sum_{i=1}^N \theta_i \geq 0$, $\theta_0 p_0 = -\sum_{i=1}^N \theta_i \mathrm{Tr}(\mathbf{Q}_i)$, and μ is a probability measure satisfying $\mathrm{supp} \mu \subset \{X \in \mathbb{R}_{sym}^{n \times n} : \mathrm{Tr}(X) = p_0\}$.

These conditions are all satisfied by the gradient Young measure generated by the rescaled sequence $\mathbf{v}^{(k)} = \nabla u^{(k)}$. In particular, the Dirac masses at \mathbf{Q}_i arise from the periodic E-inclusions and the condition $\text{Tr}(X) = p_0$ arises from the Poisson equation $\Delta u = p_0$ on the complementary set. From the basic relation between gradient Young measures and quasiconvex functions (KINDERLEHRER & PEDREGAL [31, 32]), we have that

$$\int_{\mathbb{R}^{n \times n}} \psi(X) d\nu(X) \geq \psi(0) \quad (5-2)$$

for all quasiconvex functions $\psi : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$. The notion of quasiconvexity used here is the one appropriate for second gradient (ŠVERÁK [53]). In particular, we can show that, by similar arguments as in ALLAIRE & KOHN [1], equation (5-2) holds if ψ is quadratic and is rank-one convex for symmetric rank-one matrices.

We now show that the previous restrictions (2-16) on \mathbb{K} and Θ also follow from equation (5-2). For any $X \in \mathbb{R}_{sym}^{n \times n}$, consider the quadratic function $\psi(X) = \mathbf{m} \cdot (\text{Tr}(X)X - X^2)\mathbf{m}$ for some $\mathbf{m} \in \mathbb{R}^n$. Direct calculations reveal that $\psi(X + \lambda \mathbf{n} \otimes \mathbf{n}) = \psi(X) + \lambda(\mathbf{m} \cdot X \mathbf{m} |\mathbf{n}|^2 + \text{Tr}(X)(\mathbf{n} \cdot \mathbf{m})^2 - 2(\mathbf{n} \cdot \mathbf{m})\mathbf{n} \cdot X \mathbf{m})$ is an affine function of λ for any $\mathbf{n}, \mathbf{m} \in \mathbb{R}^n$ and therefore is convex on symmetric rank-one matrices. (In fact, ψ is a null Lagrangian in this second gradient context.) An application of (5-2) to $\pm\psi$ shows that for a sequential E-inclusion (5-1),

$$\begin{aligned} 0 &= \int_{\mathbb{R}^{n \times n}} (\text{Tr}(X)X - X^2) d\nu(X) \quad (5-3) \\ &= \sum_{i=1}^N \theta_i (\text{Tr}(\mathbf{Q}_i)\mathbf{Q}_i - \mathbf{Q}_i^2) + \theta_0 \int_{\mathbb{R}^{n \times n}} (\text{Tr}(X)X - X^2) d\mu(X). \end{aligned}$$

Since the center of mass of ν is zero, we have

$$\int_{\mathbb{R}^{n \times n}} \text{Tr}(X)X d\mu(X) = p_0 \int_{\mathbb{R}^{n \times n}} X d\mu(X) = p_0 [-\sum_{i=1}^N \theta_i \mathbf{Q}_i] / \theta_0. \quad (5-4)$$

The last term in (5-3) can be bounded using Jensen's inequality

$$\int_{\mathbb{R}^{n \times n}} X^2 d\mu(X) \geq \left[\int_{\mathbb{R}^{n \times n}} X d\mu(X) \right]^2 = [-\sum_{i=1}^N \theta_i \mathbf{Q}_i]^2 / \theta_0^2. \quad (5-5)$$

Substituting equations (5-4) and (5-5) into (5-3), we obtain

$$\sum_{i=1}^N [\theta_0 \text{Tr}(\mathbf{Q}_i) + \sum_{j=1}^N \theta_j \text{Tr}(\mathbf{Q}_j)] \theta_i \mathbf{Q}_i \geq \theta_0 \sum_{i=1}^N \theta_i \mathbf{Q}_i^2 + [\sum_{i=1}^N \theta_i \mathbf{Q}_i]^2,$$

which is identical to equation (2-16). Of course, there are many other quasi-convex functions that could be used in equation (5-2) that would evidently give further restrictions on the \mathbb{K} and Θ .

As shown in forthcoming work on optimal bounds for multiphase composites (LIU [35]), the concept of a sequential E-inclusion is useful to characterize the microstructures that attain the Hashin-Shtrikman bounds. The result, in its strongest form, states that under restrictions on $\mathbf{L}_1, \dots, \mathbf{L}_N$ of the type given here, a microstructure attains the Hashin-Shtrikman bounds if and only if it is a sequential E-inclusion.

E-inclusions can be generalized to other situations. For instance, if an open bounded domain D is considered, special structures such that the overdetermined problem

$$\begin{cases} \Delta u = \sum_{i=0}^N p_i \chi_{\Omega_i} & \text{on } D, \\ \nabla \nabla u = \mathbf{Q}_i & \text{on } \Omega_i \quad \forall i = 1, \dots, N, \\ u = 0 & \text{on } \partial D \end{cases}$$

admits a solution can be defined and constructed by the counterpart of variational inequality (2-1). It is expected that these special structures have similar extremal properties as periodic E-inclusions with respect to the corresponding energy minimization problem. It is also clear that the variational inequality (2-1) can be used to construct special inclusions based on an obstacle ϕ_{per} that is *not* a piecewise quadratic function.

E-inclusions can also be used to solve problems on the effective behavior of nonlinear composites. For instance, let us consider a periodic two-phase nonlinear composite with effective properties defined by

$$I^e(\mathbf{e}) = \min_{w \in W_{per}^{1,2}(Y)} \int_Y I(\nabla w + \mathbf{e}, \mathbf{x}) d\mathbf{x} \quad \forall \mathbf{e} \in \mathbb{R}^n, \quad (5-6)$$

where the energy function $I : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ is given by

$$I(\mathbf{e}, \mathbf{x}) = \begin{cases} I_1(\mathbf{e}) & \text{if } \mathbf{x} \in \Omega, \\ \mathbf{e} \cdot \mathbf{I} \mathbf{e} & \text{if } \mathbf{x} \in Y \setminus \Omega. \end{cases}$$

Here $I_1 : \mathbb{R}^n \rightarrow \mathbb{R}$, describing the nonlinear phase on Ω , is a strictly convex but not necessarily quadratic function, and the identity matrix \mathbf{I} describes the linear phase on $Y \setminus \Omega$. If Ω is a periodic E-inclusion with matrix $\mathbf{Q} \in \mathbb{Q}$ and volume fraction θ (cf., (2-19)), the minimization problem (5-6) is explicitly solvable in terms of a linear combination of functions satisfying (2-19) in spite of the nonlinearity of $I_1(\mathbf{e})$. Essentially, the fact that ∇w is constant on Ω reduces the nonlinear part of the problem to an algebraic equation. This observation (for ellipsoids) goes back to HILL [24].

Structures that look a lot like E-inclusions are apparently seen in nature. For instance, Fig. 12 is a dark-field electron micrograph of Ni_3Ge precipitates in late stage coarsening of binary Ni-Ge alloys. The experimental conditions are described in KIM & ARDELL [30]. The transformation

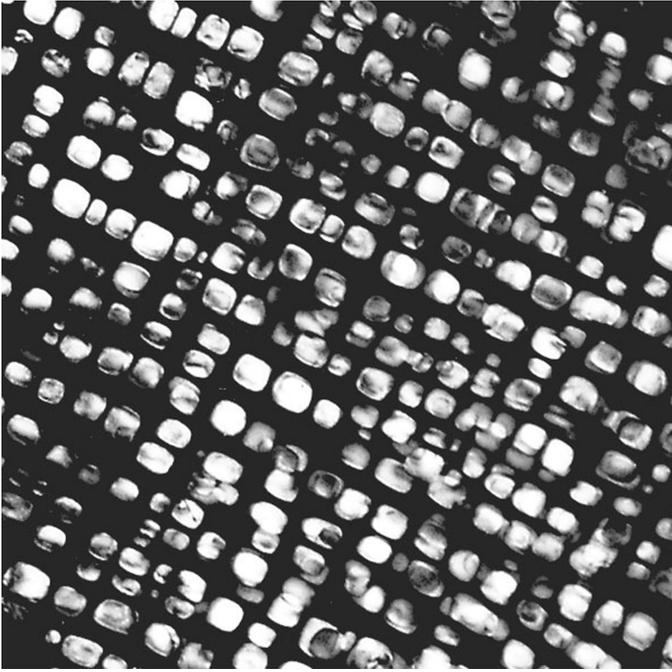


Fig. 12. *Dark-field transmission electron micrographs of the Ni_3Ge precipitates, see KIM & ARDELL [30] for the experimental conditions.*

strain is dilatational in this case and the transformation is cubic to cubic. Precipitates in this and other coarsening nickel-based superalloys form approximately periodic arrays and have shapes like those seen in Fig. 7. Like periodic E-inclusions, these precipitates become more cuboidal at higher volume fraction. In late stage coarsening it is accepted that the minimization of elastic energy, both with respect to fields as well as shapes, governs the evolution of microstructure (JOU, LEO & LOWENGRUB [25]; THORNTON, AKAIWA & VOORHEES [51]). In addition, interfacial energy plays a role in the evolution, but its influence is less important at the later stages of coarsening. E-inclusions are likely to be favored in the evolution of precipitates in these alloys since they are optimal shapes with respect to elastic energy, as shown in Section 4. To make this possible connection between E-inclusions and Ni_3Ge precipitates quantitative, one should find an estimate of the effect of the presence of interfacial energy on shape. Also, one would also need to check that the elasticity tensor of the matrix phase exceeds that of the precipitate (or generalize our results) and generalize our results to allow a cubic matrix phase.

Finally we remark that the analogy between ellipsoids and periodic E-inclusions is not perfect in the sense that $\nabla \mathbf{v}$ is uniform on the ellipsoid in problem (1-1) for *any* matrix \mathbf{P} , whereas periodic E-inclusions have this

property only for the matrix $\mathbf{P} = \mathbf{I}$, unless the tensor \mathbf{L}_2 has a special form. Nevertheless, we anticipate periodic E-inclusions can find wide applications in the theories of micromechanics, composites and fracture mechanics as does the ubiquitous *Eshelby's solution* in these fields. In the meantime, it is interesting to know if the solution $\nabla \mathbf{v}$ of problem (4-6) is uniform on a periodic E-inclusion for other matrices \mathbf{P}, \mathbf{L}_2 , subject to some additional assumption, say, the periodic E-inclusion is simply connected in one unit cell. This could be explored numerically.

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