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MICROSTRUCTURAL TOPOLOGICAL SENSITIVITIES OF THE SECOND-ORDER MACROSCOPIC MODEL FOR WAVES IN PERIODIC MEDIA*

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Abstract. We consider scalar waves in periodic media through the lens of a second-order effective, i.e., macroscopic description, and we aim to compute the sensitivities of the germane effective parameters due to topological perturbations of a microscopic unit cell. Specifically, our analysis focuses on the tensorial coefficients in the governing mean field equation—including both the leading order (i.e., quasi-static) terms, and their second-order companions bearing the effects of incipient wave dispersion. The results demonstrate that the sought sensitivities are computable in terms of (i) three unit cell solutions used to formulate the unperturbed macroscopic model; (ii) two adoint-field solutions driven by the mass density variation inside the unperturbed unit cell; and (iii) the usual polarization tensor, appearing in the related studies of nonperiodic media, that synthesizes the geometric and constitutive features of a point-like perturbation. The proposed developments may be useful toward (a) the design of periodic media to manipulate macroscopic waves via the microstructure-generated effects of dispersion and anisotropy, and (b) subwavelength sensing of periodic defects or perturbations.

Key words. waves in periodic media, second-order homogenization, topological sensitivity, periodic perturbations

AMS subject classifications. 35B27, 35J05, 74H10, 74Q10

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1. Introduction. Over the past decade, waves in periodic media have been the subject of mounting attention owing to an exceeding ability of periodic structures to provide cloaking, noise control, and subwavelength imaging [21, 29, 20]. Fundamentally, the latter derive from the underpinning phenomena of frequency-dependent anisotropy, multiple solution branches, and band gaps [9] that can be manipulated through a suitable design of the unit stencil. Some of the above and related effects, including cloaking and a negative index of refraction, are often achieved at long wavelengths [13]—extending beyond the periodicity cell. This poses the question of mathematical tools that can aid the design, via, e.g., topology optimization [25], of periodic "microstructures" toward gaining a desired macroscopic effect.

In this vein, our study aims to distill the sensitivity of wave motion in a periodic composite due to small topological alterations of its unit cell. In other words, we consider perturbations that are inherently periodic according to the germane lattice. With reference to a (dispersive) field equation governing the *effective,* i.e., *macroscopic* wave motion, we specifically seek to compute the so-called topological sensitivities (TSs) of the coefficients in the field equation with respect to the nucleation

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of a vanishing inhomogeneity inside the microscopic unit cell. The concept of TS was introduced in the late 1990s (see [24] for references), and can be described as follows. For a given boundary value problem, one considers (in the classical sense, an individual) topological perturbation of vanishing size a at some point $\boldsymbol{z}$ inside the reference domain, and seeks the TS of any relevant quantity J as an a-independent factor in the leading-order asymptotic expansion of J as $a \to 0$. In this way the map $\mathrm{TS}(\boldsymbol{z})$, which is typically inexpensive to compute, helps drive the topological optimization procedure by highlighting the region(s) where medium alterations may be most beneficial toward increasing or decreasing J.

With the above goal in mind, the natural first step in the analysis is to identify the field equation that governs the macroscopic wave motion in a "microstructured" periodic medium. Such an effective model should preferably include the effects of (anisotropic) wave dispersion to cater for intended applications. To this end, we deploy the framework of two-scale homogenization [6] and pursue the expansion up to the second order [4, 27], rather than deploying the competing (physics-based) approaches such as the Mindlin's second-gradient theory [22, 5] or the Willis' concept of effective constitutive relationships [28, 23]. The key advantage of the adopted approach resides in the fact that the two-scale paradigm produces a set of unit cell problems from which the homogenized coefficients are then computed. These cell problems, endowed with periodic boundary conditions, are (i) of elliptic type and (ii) well-posed, thus facilitating a systematic derivation of the germane small-perturbation asymptotics by building upon the related works on conductivity-like problems [10, 2, 7].

To facilitate the discussion and to maintain a clear link with prior works [4, 27], we interpret the scalar wave equation within the framework of (elastic) antiplane shear waves. Notwithstanding such a choice, the ensuing analysis applies to a much wider range of physical problems (see, e.g., [18, Table 1]), which notably include the transverse modes of electromagnetic wave propagation. More generally, our work extends the previous TS analyses of periodic media—performed in the context of elastostatics and structural shape optimization [14, 3, 26]—to dynamic, i.e., *wave motion* problems described via *second-order homogenization*. Equivalently, this study can be seen as a follow-up to the small-inclusion asymptotic analyses underpinning the (approximate) effective description of low-volume fraction dilutions [12] and two-phase periodic composites; e.g., [2, 18]. In principle, the idea of topological perturbation can also be applied to the (leading-order) effective description [11] of higher, i.e., "optical" solution branches for a given periodic medium; the latter topic is, however, beyond the scope of this study.

The paper is organized as follows. Section 2 provides a review of the relevant two-scale homogenization results, and introduces topological perturbations of the unit cell. Section 3 derives the necessary asymptotics for a cascade of the unit cell problems, and introduces the polarization tensor that arises in the analysis. Our main result, Theorem 5, which provides the TS expressions for the coefficients featured by the effective, i.e., macroscopic, field equation, is presented and discussed in section 4. Section 5 is dedicated to some auxiliary results that were delayed for better readability, while section 6 provides the proof of Theorem 5. Section 7 illustrates via numerical simulations how the obtained TS results can be used toward *subwavelength sensing*, where the information on long-wavelength (anisotropic) dispersion can be used to localize periodic defects inside the unit cell, due to, e.g., a manufacturing error. Finally, section 8 highlights the key contributions of our work.

2. Preliminaries.

2.1. Two-scale homogenization framework. In the context of two-dimensional antiplane elasticity, we consider a reference biperiodic medium whose periodicity cell $Y = (0,1) \times (0,\alpha) \subset \mathbb{R}^2$, $\alpha = O(1)$, is endowed with smooth $Y \to \mathbb{R}$ distributions of the shear modulus $\mu(\boldsymbol{x})$ and mass density $\rho(\boldsymbol{x})$. Note that the latter restriction can, in principle, be weakened; in particular, piecewise-smooth characteristics may be considered instead; see Remark 3. Letting $\varepsilon > 0$ be a small perturbation parameter, we next consider an εY-periodic medium endowed with the shear modulus $\mu_\varepsilon(\boldsymbol{x}) := \mu(\boldsymbol{x}/\varepsilon)$ and mass density $\rho_\varepsilon(\boldsymbol{x}) := \rho(\boldsymbol{x}/\varepsilon)$. A time-harmonic antiplane shear wave propagating in such a medium, described in terms of the transverse displacement $u = u_\varepsilon(\boldsymbol{x})e^{-\mathrm{i}\omega t}$, obeys the field equation

$$\operatorname{div}\big(\mu_\varepsilon \boldsymbol{\nabla} u_\varepsilon\big) + \rho_\varepsilon \omega^2 u_\varepsilon = 0, \tag{1}$$

and admits a two-scale expansion [6, 27] of the form

$$u_\varepsilon(\boldsymbol{x}) := u_0(\boldsymbol{x},\boldsymbol{y}) + \varepsilon u_1(\boldsymbol{x},\boldsymbol{y}) + \varepsilon^2 u_2(\boldsymbol{x},\boldsymbol{y}) + \varepsilon^3 u_3(\boldsymbol{x},\boldsymbol{y}) + o(\varepsilon^3), \tag{2}$$

whose coefficients u_0, u_1, u_2, u_3 are functions of the "slow" variable $\boldsymbol{x} \in \mathbb{R}^2$ and the "fast" variable $\boldsymbol{y} := \boldsymbol{x}/\varepsilon \in Y$, computable as

$$\begin{aligned}
u_0(\boldsymbol{x},\boldsymbol{y}) &= U_0(\boldsymbol{x}),\\
u_1(\boldsymbol{x},\boldsymbol{y}) &= U_1(\boldsymbol{x}) + \boldsymbol{P}(\boldsymbol{y})\cdot\boldsymbol{\nabla} U_0(\boldsymbol{x}),\\
u_2(\boldsymbol{x},\boldsymbol{y}) &= U_2(\boldsymbol{x}) + \boldsymbol{P}(\boldsymbol{y})\cdot\boldsymbol{\nabla} U_1(\boldsymbol{x}) + \boldsymbol{Q}(\boldsymbol{y}):\boldsymbol{\nabla}^2 U_0(\boldsymbol{x}),\\
u_3(\boldsymbol{x},\boldsymbol{y}) &= U_3(\boldsymbol{x}) + \boldsymbol{P}(\boldsymbol{y})\cdot\boldsymbol{\nabla} U_2(\boldsymbol{x}) + \boldsymbol{Q}(\boldsymbol{y}):\boldsymbol{\nabla}^2 U_1(\boldsymbol{x}) + \boldsymbol{R}(\boldsymbol{y}):\boldsymbol{\nabla}^3 U_0(\boldsymbol{x}),
\end{aligned} \tag{3}$$

where U_j are the mean displacement fields defined by $U_j(\boldsymbol{x}) = \langle u_j\rangle(\boldsymbol{x})$, $\langle\cdot\rangle$ denotes the unit cell average computed with respect to the fast coordinate, i.e.,

$$\langle f\rangle(\boldsymbol{x}) = |Y|^{-1}\int_Y f(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}V(\boldsymbol{y}); \tag{4}$$

":" signifies the *scalar product* between two nth-order tensors ($n \geqslant 2$); and $\boldsymbol{P}, \boldsymbol{Q}, \boldsymbol{R}$ are the so-called *unit cell functions* defined below. In (3) and thereafter, the gradient operator $\boldsymbol{\nabla}$ and its powers $\boldsymbol{\nabla}^j = \boldsymbol{\nabla}(\boldsymbol{\nabla}^{j-1})$ act "to the right", e.g., $(\boldsymbol{\nabla}\boldsymbol{A})_{ijk} = \partial_i A_{jk}$ for a second-order tensor field $\boldsymbol{A}$. Accordingly, the divergence operator is understood in a commensurate way, e.g., $(\operatorname{div}\boldsymbol{A})_k = \partial_j A_{jk}$.

Cell functions and homogenized coefficients. The tensor-valued cell functions $\boldsymbol{P} : Y \to \mathbb{R}^2$, $\boldsymbol{Q} : Y \to (\mathbb{R}^2)^2$, and $\boldsymbol{R} : Y \to (\mathbb{R}^2)^3$ solve the well-posed [6] recursive cell problems

$$\left.\begin{aligned}
\operatorname{div}\big[\mu(\boldsymbol{I} + \boldsymbol{\nabla}\boldsymbol{P})\big] &= \boldsymbol{0} \qquad \text{in } Y,\\
\mu\,\boldsymbol{n}\cdot\boldsymbol{\nabla}\boldsymbol{P} \quad &Y\text{-periodic}, \quad \langle\boldsymbol{P}\rangle = \boldsymbol{0},
\end{aligned}\right\} \tag{5a}$$

$$\left.\begin{aligned}
\operatorname{div}\big[\mu(\boldsymbol{I}\otimes\boldsymbol{P} + \boldsymbol{\nabla}\boldsymbol{Q})\big] + \mu(\boldsymbol{I} + \boldsymbol{\nabla}\boldsymbol{P}) - \rho\frac{\boldsymbol{\mu}^0}{\varrho^0} &= \boldsymbol{0} \qquad \text{in } Y,\\
\mu\,\boldsymbol{n}\cdot\big(\boldsymbol{I}\otimes\boldsymbol{P} + \boldsymbol{\nabla}\boldsymbol{Q}\big) \quad &Y\text{-periodic}, \quad \langle\boldsymbol{Q}\rangle = \boldsymbol{0},
\end{aligned}\right\} \tag{5b}$$

$$\left.\begin{aligned}
\operatorname{div}\big[\mu(\boldsymbol{I}\otimes\boldsymbol{Q} + \boldsymbol{\nabla}\boldsymbol{R})\big] + \mu(\boldsymbol{I}\otimes\boldsymbol{P} + \boldsymbol{\nabla}\boldsymbol{Q})&\\
- \rho\boldsymbol{P}\otimes\frac{\boldsymbol{\mu}^0}{\varrho^0} + \rho\Big[\frac{\boldsymbol{\varrho}^1}{\varrho^0}\otimes\frac{\boldsymbol{\mu}^0}{\varrho^0} - \frac{\boldsymbol{\mu}^1}{\varrho^0}\Big] &= \boldsymbol{0} \qquad \text{in } Y,\\
\mu\,\boldsymbol{n}\cdot\big(\boldsymbol{I}\otimes\boldsymbol{Q} + \boldsymbol{\nabla}\boldsymbol{R}\big) \quad &Y\text{-periodic}, \quad \langle\boldsymbol{R}\rangle = \boldsymbol{0}.
\end{aligned}\right\} \tag{5c}$$

In (5), $\varrho^0 \in \mathbb{R}$, $\boldsymbol{\varrho}^1 \in \mathbb{R}^2$, $\boldsymbol{\mu}^0 \in (\mathbb{R}^2)^2$, $\boldsymbol{\mu}^1 \in (\mathbb{R}^2)^3$ are constant tensorial quantities given by

$$\begin{aligned} &\text{(a)}\ \ \varrho^0 = \big\langle \rho \big\rangle, && \text{(c)}\ \ \boldsymbol{\mu}^0 = \big\langle \mu(\boldsymbol{\nabla} \boldsymbol{P} + \boldsymbol{I}) \big\rangle_{\mathrm{sym}}, \\ &\text{(b)}\ \ \boldsymbol{\varrho}^1 = \big\langle \rho \boldsymbol{P} \big\rangle, && \text{(d)}\ \ \boldsymbol{\mu}^1 = \big\langle \mu(\boldsymbol{\nabla} \boldsymbol{Q} + \boldsymbol{I} \otimes \boldsymbol{P}) \big\rangle_{\mathrm{sym}}. \end{aligned} \tag{6}$$

Here, the subscript "sym" indicates tensor symmetrization obtained by averaging over all component index permutations. In particular, for a tensor $\boldsymbol{A}$ of order n and a given n-tuple of indices $I \in \{1,2\}^n$, we have

$$\big(\boldsymbol{A}_{\mathrm{sym}}\big)_I = \frac{1}{n!} \sum_{\sigma \in \Pi_n} A_{\sigma(I)}, \tag{7}$$

where Π_n denotes the set of all permutations $\sigma(I)$. In the following, we will also make use of the higher-order "descendants" of (6), namely, $\boldsymbol{\varrho}^2 \in (\mathbb{R}^2)^2$ and $\boldsymbol{\mu}^2 \in (\mathbb{R}^2)^4$, defined by

$$\text{(a)}\ \ \boldsymbol{\varrho}^2 = \big\langle \rho \boldsymbol{Q} \big\rangle_{\mathrm{sym}}, \qquad \text{(b)}\ \ \boldsymbol{\mu}^2 = \big\langle \mu(\boldsymbol{\nabla} \boldsymbol{R} + \boldsymbol{I} \otimes \boldsymbol{Q}) \big\rangle_{\mathrm{sym}}. \tag{8}$$

One may note that the entries in (6) obey the following interrelationship, which, in particular, causes the bracketed factor of ρ in (5c) to vanish.

LEMMA 1. *The tensorial quantities in* (6) *satisfy the "reciprocity" relationship* $\varrho^0 \boldsymbol{\mu}^1 = \big(\boldsymbol{\varrho}^1 \otimes \boldsymbol{\mu}^0\big)_{\mathrm{sym}}$.

Proof. The claim is verified by (i) taking the tensor product of $\boldsymbol{Q}$ and (5a) and of $\boldsymbol{P}$ and (5b), (ii) subtracting the obtained equalities, (iii) integrating over Y, and (iv) symmetrizing the resulting tensor equality in the sense of (7). ∎

Cell problems, weak formulation. Let $\boldsymbol{\mathcal{V}}_p$ denote the function spaces of (pth-order tensor-valued, zero-mean, Y-periodic functions) given by

$$\begin{aligned} \mathcal{V} := \boldsymbol{\mathcal{V}}_0 &= \big\{ w \in H^1\big(Y; \mathbb{R}\big),\ \langle w \rangle_Y = 0,\ w\ Y\text{-periodic} \big\}, \\ \boldsymbol{\mathcal{V}}_p &= \big\{ \boldsymbol{w} \in H^1\big(Y; (\mathbb{R}^2)^p\big),\ \langle \boldsymbol{w} \rangle_Y = 0,\ \boldsymbol{w}\ Y\text{-periodic} \big\} \quad \text{for } p \geq 1 \end{aligned} \tag{9}$$

with the implicit convention that $\boldsymbol{\mathcal{V}}$ (without subscript) refers to $\boldsymbol{\mathcal{V}}_p$ for some unspecified p. In what follows, we will also denote by $\boldsymbol{w}^{\mathrm{T}}$ the reversal of tensor indexes; for instance, one has $(\boldsymbol{w}^{\mathrm{T}})_{ijkl} = (\boldsymbol{w})_{lkji}$ for a fourth-order tensor $\boldsymbol{w}$. In this setting, each of the cell problems in (5) has a weak formulation. On introducing the bilinear form

$$\big\langle\!\big\langle \boldsymbol{w}, \boldsymbol{v} \big\rangle\!\big\rangle_X^{\eta} = \int_X \eta\, (\boldsymbol{\nabla} \boldsymbol{w})^{\mathrm{T}} \cdot \boldsymbol{\nabla} \boldsymbol{v}\, \mathrm{d}V \tag{10}$$

associated with elastic strain energy for some domain $X \subset \mathbb{R}^2$ and shear modulus η, tensor-valued cell functions $\boldsymbol{P} \in \boldsymbol{\mathcal{V}}_1$, $\boldsymbol{Q} \in \boldsymbol{\mathcal{V}}_2$, and $\boldsymbol{R} \in \boldsymbol{\mathcal{V}}_3$ can be shown to solve the weak problems

$$\big\langle\!\big\langle w, \boldsymbol{P} \big\rangle\!\big\rangle_Y^{\mu} = -\boldsymbol{F}(w) \qquad \text{for all } w \in \mathcal{V}, \tag{11a}$$

$$\big\langle\!\big\langle w, \boldsymbol{Q} \big\rangle\!\big\rangle_Y^{\mu} = \boldsymbol{J}(w, \boldsymbol{P}) + \boldsymbol{K}^Q(w) - \boldsymbol{L}^Q(w) \qquad \text{for all } w \in \mathcal{V}, \tag{11b}$$

$$\big\langle\!\big\langle w, \boldsymbol{R} \big\rangle\!\big\rangle_Y^{\mu} = \boldsymbol{J}(w, \boldsymbol{Q}) + \boldsymbol{K}^R(w) - \boldsymbol{L}^R(w) \qquad \text{for all } w \in \mathcal{V}. \tag{11c}$$

The right-hand sides of (11a)–(11c) involve the bilinear form $\boldsymbol{J}$, defined by

$$\boldsymbol{J}(\boldsymbol{w},\boldsymbol{v}) = \int_Y \mu\big(\boldsymbol{w}^{\mathrm{T}}\otimes\boldsymbol{\nabla}\boldsymbol{v} - (\boldsymbol{\nabla}\boldsymbol{w})^{\mathrm{T}}\otimes\boldsymbol{v}\big)\,\mathrm{d}V \tag{12}$$

and the linear functionals

(13)

$$\begin{aligned}
\boldsymbol{F}(\boldsymbol{w}) &= \int_Y \mu(\boldsymbol{\nabla}\boldsymbol{w})^{\mathrm{T}}\,\mathrm{d}V \;= -\boldsymbol{J}(\boldsymbol{w},1),\\
\boldsymbol{K}^Q(\boldsymbol{w}) &= \int_Y \mu\boldsymbol{w}^{\mathrm{T}}\otimes\boldsymbol{I}\,\mathrm{d}V, \qquad & \boldsymbol{K}^R(\boldsymbol{w}) &= \int_Y \mu\boldsymbol{w}^{\mathrm{T}}\otimes\boldsymbol{I}\otimes\boldsymbol{P}\,\mathrm{d}V,\\
\boldsymbol{L}^Q(\boldsymbol{w}) &= \int_Y \rho\boldsymbol{w}^{\mathrm{T}}\otimes\frac{\boldsymbol{\mu}^0}{\varrho^0}\,\mathrm{d}V, \qquad & \boldsymbol{L}^R(\boldsymbol{w}) &= \int_Y \rho\boldsymbol{w}^{\mathrm{T}}\otimes\frac{\boldsymbol{\mu}^0}{\varrho^0}\otimes\boldsymbol{P}\,\mathrm{d}V.
\end{aligned}$$

Although the weak problems (11) involve scalar test functions (reflecting the fact that the problems governing each scalar component of $\boldsymbol{P},\boldsymbol{Q},\boldsymbol{R}$ are uncoupled), it will be convenient in the following to extend (11) together with the affiliated linear and bilinear forms to tensor-valued test functions $\boldsymbol{w}$—a need to which definitions (10), (12), and (13) cater. The definition (12) of $\boldsymbol{J}$ further implies that, for any pair $(\boldsymbol{v},\boldsymbol{w})$ of scalar or tensor-valued functions,

$$\boldsymbol{J}(\boldsymbol{w},\boldsymbol{v}) \;=\; -\boldsymbol{J}^{\mathrm{T}}(\boldsymbol{v},\boldsymbol{w}). \tag{14}$$

With reference to (13), we note that the homogenized shear moduli can be written in terms of the functionals $\boldsymbol{F}$ and $\boldsymbol{K}^Q$ as

$$\boldsymbol{\mu}^0 = |Y|^{-1}\big(\boldsymbol{F}(\boldsymbol{P}) + |Y|\langle\mu\rangle\boldsymbol{I}\big)_{\mathrm{sym}}, \tag{15a}$$

$$\boldsymbol{\mu}^1 = |Y|^{-1}\big(\boldsymbol{F}(\boldsymbol{Q}) + \boldsymbol{K}^Q(\boldsymbol{P})\big)_{\mathrm{sym}}, \tag{15b}$$

$$\boldsymbol{\mu}^2 = |Y|^{-1}\big(\boldsymbol{F}(\boldsymbol{R}) + \boldsymbol{K}^Q(\boldsymbol{Q})\big)_{\mathrm{sym}}. \tag{15c}$$

Mean field. Let $U(\boldsymbol{x})$ denote the (macroscopic) mean field associated with u_ε, defined by

$$\begin{aligned}
U(\boldsymbol{x}) &= \big\langle\, u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \varepsilon^3 u_3 + o(\varepsilon^3)\,\big\rangle\\
&= U_0(\boldsymbol{x}) + \varepsilon U_1(\boldsymbol{x}) + \varepsilon^2 U_2(\boldsymbol{x}) + \varepsilon^3 U_3(\boldsymbol{x}) + o(\varepsilon^3).
\end{aligned}$$

Its $O(\varepsilon^3)$ approximation, $U^{(3)} := U^0 + \varepsilon U_1 + \varepsilon^2 U_2 + \varepsilon^3 U_3$, can, in particular, be shown [27] to satisfy the homogenized field equation

$$\boldsymbol{\mu}^0 : \boldsymbol{\nabla}^2 U^{(3)} + \varepsilon^2 \boldsymbol{\mu}^2 : \boldsymbol{\nabla}^4 U^{(3)} + \omega^2\big(\,\varrho^0 U^{(3)} + \varepsilon^2 \boldsymbol{\varrho}^2 : \boldsymbol{\nabla}^2 U^{(3)}\big) = o(\varepsilon^3), \tag{16}$$

where ϱ^0, $\boldsymbol{\mu}^0$, $\boldsymbol{\varrho}^2$, and $\boldsymbol{\mu}^2$ are given by (6) and (8). Note that the contribution of $\boldsymbol{\varrho}^1$ and $\boldsymbol{\mu}^1$ in (16) vanishes as a consequence of Lemma 1, while the $o(\varepsilon^3)$ remainder (instead of expected $O(\varepsilon^3)$ residual) stems from the analogous relationship linking $\boldsymbol{\varrho}^3$ and $\boldsymbol{\mu}^3$ to their lower-order companions.

2.2. Perturbed cell configuration. Let $\Delta\mu > -\min_{\boldsymbol{x}\in Y}\mu(\boldsymbol{x})$ and $\Delta\rho > -\min_{\boldsymbol{x}\in Y}\rho(\boldsymbol{x})$ be prescribed material contrasts. We now introduce at some $\boldsymbol{z}\in Y$ a small inhomogeneity $B_a = \boldsymbol{z} + a\mathcal{B}$ of size a and shape $\mathcal{B}$, endowed with the shear modulus $\mu+\Delta\mu$ and mass density $\rho+\Delta\rho$. The material characteristics of the perturbed

cell Y_a are, hence, $\mu_a = \mu + \chi(B_a)\Delta\mu$ and $\rho_a = \rho + \chi(B_a)\Delta\rho$, where $\chi(\cdot)$ denotes the characteristic function of a perturbation. The size a is assumed to be sufficiently small so that $B_a \Subset Y$, whereby $\mu_a = \mu$ and $\rho_a = \rho$ in the vicinity of ∂Y. We use notations $\langle\!\langle \boldsymbol{w}, \boldsymbol{v} \rangle\!\rangle_Y^{\mu_a}$, $\boldsymbol{P}_a$, etc., and $\boldsymbol{J}_a$, $\boldsymbol{K}_a^Q$, etc. whenever cell problems and effective characteristics are considered for the perturbed cell. The weak cell problems (11a)–(11c) for the perturbed cell then read

$$\langle\!\langle w, \boldsymbol{P}_a \rangle\!\rangle_Y^{\mu_a} = -\boldsymbol{F}_a(w) \qquad \text{for all } w \in \mathcal{V}, \tag{17a}$$

$$\langle\!\langle w, \boldsymbol{Q}_a \rangle\!\rangle_Y^{\mu_a} = \boldsymbol{J}_a(w, \boldsymbol{P}_a) + \boldsymbol{K}_a^Q(w) - \boldsymbol{L}_a^Q(w) \qquad \text{for all } w \in \mathcal{V}, \tag{17b}$$

$$\langle\!\langle w, \boldsymbol{R}_a \rangle\!\rangle_Y^{\mu_a} = \boldsymbol{J}_a(w, \boldsymbol{Q}_a) + \boldsymbol{K}_a^R(w) - \boldsymbol{L}_a^R(w) \qquad \text{for all } w \in \mathcal{V}. \tag{17c}$$

Moreover, introducing the cell function perturbations $\boldsymbol{p}_a := \boldsymbol{P}_a - \boldsymbol{P}$, $\boldsymbol{q}_a := \boldsymbol{Q}_a - \boldsymbol{Q}$, and $\boldsymbol{r}_a := \boldsymbol{R}_a - \boldsymbol{R}$ and combining problems (17a)–(17c) with problems (11a)–(11c), we obtain the following identities:

$$\langle\!\langle w, \boldsymbol{p}_a \rangle\!\rangle_Y^{\mu} + \langle\!\langle w, \boldsymbol{P}_a \rangle\!\rangle_{B_a}^{\Delta\mu} = -\Delta\boldsymbol{F}_a(w)$$

$$\text{for all } w \in \mathcal{V}, \tag{18a}$$

$$\langle\!\langle w, \boldsymbol{q}_a \rangle\!\rangle_Y^{\mu} + \langle\!\langle w, \boldsymbol{Q}_a \rangle\!\rangle_{B_a}^{\Delta\mu} = \Delta\boldsymbol{J}_a(w, \boldsymbol{P}_a) + \boldsymbol{J}(w, \boldsymbol{p}_a) + \Delta\boldsymbol{K}_a^Q(w) - \Delta\boldsymbol{L}_a^Q(w)$$

$$\text{for all } w \in \mathcal{V}, \tag{18b}$$

$$\langle\!\langle w, \boldsymbol{r}_a \rangle\!\rangle_Y^{\mu} + \langle\!\langle w, \boldsymbol{R}_a \rangle\!\rangle_{B_a}^{\Delta\mu} = \Delta\boldsymbol{J}_a(w, \boldsymbol{Q}_a) + \boldsymbol{J}(w, \boldsymbol{q}_a) + \Delta\boldsymbol{K}_a^R(w) - \Delta\boldsymbol{L}_a^R(w)$$

$$\text{for all } w \in \mathcal{V}, \tag{18c}$$

$$\Delta\boldsymbol{F}_a(\cdot) := \boldsymbol{F}_a(\cdot) - \boldsymbol{F}(\cdot),\ \Delta\boldsymbol{J}_a(\cdot, \boldsymbol{v}_a) := \boldsymbol{J}_a(\cdot, \boldsymbol{v}_a) - \boldsymbol{J}(\cdot, \boldsymbol{v}_a).$$

In particular, one has

$$\Delta\boldsymbol{F}_a(\boldsymbol{w}) = \Delta\mu \int_{B_a} (\boldsymbol{\nabla}\boldsymbol{w})^{\mathrm{T}} \,\mathrm{d}V. \tag{19}$$

2.3. Topological sensitivity of the effective properties. Let $f = f(\mu, \rho)$ stand for any of the effective tensors defined in (6) and (8) for the reference unit cell Y and, similarly, let $f_a = f(\mu_a, \rho_a)$ denote its companion computed for Y_a. Our main goal is to determine the *TS* $\mathcal{D}f(\boldsymbol{z})$ of f due to nucleation of a small inhomogeneity B_a at $\boldsymbol{z} \in Y$, defined through the expansion

$$f_a \;=\; f \,+\, \upsilon(a)\, \mathcal{D}f(\boldsymbol{z}) + o(\upsilon(a)) \quad \text{as} \quad a \to 0, \tag{20}$$

where the homogeneous scaling function $\upsilon(a)$ is to be determined. In general $\mathcal{D}f(\boldsymbol{z})$ is a function of the nucleation locus $\boldsymbol{z}$, the shape $\mathcal{B}$ of B_a, and the material properties of Y and Y_a. The latter dependence is both explicit (through definitions (6) and (8)) and implicit (through the cell functions solving (5)).

3. Cell solution asymptotics. The derivation of topological expansion (20) for the effective properties featured in the mean field equation (16) is predicated on knowing the asymptotic behavior of the cell functions as $a \to 0$, a prerequisite to which this section is devoted. To this end, the weak problems (11) for the perturbed cell are first reformulated as volume integral equations (VIEs), which are then expanded about $a \to 0$. Such an approach facilitates the computation of the sought asymptotics, as the geometrical support of the volume integral operator is the vanishing inhomogeneity B_a.

3.1. First cell problem.

Volume integral equation. Let $G(\cdot,\boldsymbol{x})$ denote the periodic Green's function for the (unperturbed) cell Y, i.e., the (Y-periodic and zero-mean) field created by a unit point source at $\boldsymbol{x}\in Y$, whereby

$$\begin{aligned} -\mathrm{div}_1(\mu\boldsymbol{\nabla}_1 G(\cdot,\boldsymbol{x})) &= \delta(\cdot-\boldsymbol{x}) \qquad \text{in } Y,\\ \big\langle G(\cdot,\boldsymbol{x})\big\rangle = 0, \qquad & G(\cdot,\boldsymbol{x}) \ \text{ and } \ \mu\,\boldsymbol{n}\cdot\boldsymbol{\nabla}_1 G(\cdot,\boldsymbol{x}) \quad Y-\text{periodic}, \end{aligned} \tag{21}$$

where div_1 and $\boldsymbol{\nabla}_1$ imply differentiation with respect to the first argument. The solution of (21) can be conveniently decomposed as

$$G(\cdot,\boldsymbol{x}) \;=\; G_\infty(\cdot-\boldsymbol{x};\mu(\boldsymbol{x})) \,+\, G_{\mathrm{c}}(\cdot,\boldsymbol{x}), \qquad\qquad G_\infty(\boldsymbol{r};\eta) = -\frac{1}{2\pi\eta}\ln|\boldsymbol{r}|, \tag{22}$$

where $G_\infty(\cdot;\eta)$ solves $-\mathrm{div}\left(\eta\boldsymbol{\nabla}G_\infty\right)=\delta(\cdot)$ (i.e., $G_\infty(\cdot;\eta)$ is the fundamental solution for an infinite homogeneous medium with shear modulus η) while the complementary part G_{c} is an $H^1(Y)$ function.

On testing the first equation in (21) by a function $\boldsymbol{w}\in\boldsymbol{\mathcal{V}}\cap C^1(\omega_{\boldsymbol{x}})$ (where $\omega_{\boldsymbol{x}}\Subset Y$ is a neighborhood of $\boldsymbol{x}$) and applying the first Green's identity to the resulting left-hand side, the Green's function is seen to verify

$$\big\langle\!\!\big\langle G(\cdot,\boldsymbol{x}),\boldsymbol{w}\big\rangle\!\!\big\rangle_Y^{\mu} = \boldsymbol{w}(\boldsymbol{x}), \qquad \boldsymbol{x}\in Y,\ \boldsymbol{w}\in\boldsymbol{\mathcal{V}}\cap C^1(\omega_x). \tag{23}$$

The assumed smoothness of μ ensures the interior regularity of $\boldsymbol{P}$ solving (5a), which in turn allows us to use $\boldsymbol{w}=\boldsymbol{P}$ in (23) (see also Remark 3 on the case of piecewise-smooth background material). We can, in addition, set $w=G(\cdot,\boldsymbol{x})$ in (11a) (the resulting integrals being well-defined although $G(\cdot,\boldsymbol{x})\notin\mathcal{V}$). Performing these operations shows that $\boldsymbol{P}$ admits the explicit representation

$$\boldsymbol{P}(\boldsymbol{x}) = -\boldsymbol{F}(G(\cdot,\boldsymbol{x})), \qquad \boldsymbol{x}\in Y. \tag{24}$$

Similar arguments are applicable to the perturbed cell function $\boldsymbol{P}_a$, which solves (17a) and satisfies the smoothness requirement in (23) for $\boldsymbol{x}\in B_a\cup(Y\setminus\overline{B_a})$. Using (23) with $\boldsymbol{w}=\boldsymbol{P}_a$ gives

$$\big\langle\!\!\big\langle G(\cdot,\boldsymbol{x}),\boldsymbol{P}_a\big\rangle\!\!\big\rangle_Y^{\mu_a} = \boldsymbol{P}_a(\boldsymbol{x}) + \big\langle\!\!\big\langle G(\cdot,\boldsymbol{x}),\boldsymbol{P}_a\big\rangle\!\!\big\rangle_{B_a}^{\Delta\mu}, \qquad \boldsymbol{x}\in B_a\cup(Y\setminus\overline{B_a}).$$

Combining the above equality and the weak problem (17a) with $w=G(\cdot,\boldsymbol{x})$ and representation (24), the restriction of $\boldsymbol{P}_a$ to B_a is found to satisfy the VIE

$$\big(\mathcal{I}+\mathcal{L}_a\big)\boldsymbol{P}_a(\boldsymbol{x}) = \boldsymbol{P}(\boldsymbol{x}) - \Delta\boldsymbol{F}_a(G(\cdot,\boldsymbol{x})), \qquad \boldsymbol{x}\in B_a, \tag{25}$$

where $\Delta\boldsymbol{F}_a$ is given by (19) and the integral operator $\mathcal{L}_a : H^1(B_a)\to H^1(B_a)$ is defined as

$$\mathcal{L}_a f(\boldsymbol{x}) = \big\langle\!\!\big\langle G(\cdot,\boldsymbol{x}),f\big\rangle\!\!\big\rangle_{B_a}^{\Delta\mu} \;=\; \Delta\mu\int_{B_a}\boldsymbol{\nabla}_1 G(\boldsymbol{y},\boldsymbol{x})\cdot\boldsymbol{\nabla}f(\boldsymbol{y})\,\mathrm{d}V(\boldsymbol{y}).$$

Then, extending (25) to $\boldsymbol{x}\in Y\setminus\overline{B_a}$ yields an explicit representation formula for $\boldsymbol{P}_a$ outside of B_a.

Asymptotic expansion of the first cell solution. By analogy with the small-inclusion asymptotic expansions for simpler two-dimensional problems [7, 10], we introduce scaled coordinates for points $\boldsymbol{x} \in B_a$ such that

$$\boldsymbol{x} = \boldsymbol{z} + a\bar{\boldsymbol{x}}, \qquad \mathrm{d}V(\boldsymbol{x}) = a^2\, \mathrm{d}V(\bar{\boldsymbol{x}}),$$

and assume the following ansatz for the expansion of $\boldsymbol{P}_a$ inside B_a (hereon called the *inner expansion*):

$$\boldsymbol{P}_a(\boldsymbol{x}) = \boldsymbol{P}(\boldsymbol{z}) + a\boldsymbol{P}_1(\bar{\boldsymbol{x}}) + o(a), \qquad \boldsymbol{x} \in B_a. \tag{26}$$

The governing (volume integral) equation for $\boldsymbol{P}_1$ is then sought by inserting the above ansatz into (25), expanding the resulting equation about $a = 0$, and retaining the leading-order contribution. This approach relies on the following expansions being verified by the Green's function:

$$G(\boldsymbol{y}, \boldsymbol{x}) = G_\infty\big(\bar{\boldsymbol{y}} - \bar{\boldsymbol{x}}; \mu(\boldsymbol{z})\big) - \frac{1}{2\pi\mu(\boldsymbol{z})} \ln a + O(1), \tag{27a}$$

$$\boldsymbol{\nabla}_1 G(\boldsymbol{y}, \boldsymbol{x}) = a^{-1} \boldsymbol{\nabla} G_\infty\big(\bar{\boldsymbol{y}} - \bar{\boldsymbol{x}}; \mu(\boldsymbol{z})\big) + O(1), \tag{27b}$$

and also uses the Taylor expansion $\boldsymbol{P}(\boldsymbol{x}) = \boldsymbol{P}(\boldsymbol{z}) + a\bar{\boldsymbol{x}}\cdot\boldsymbol{\nabla}\boldsymbol{P}(\boldsymbol{z}) + o(a)$ of the background cell solution $\boldsymbol{P}$ (which is valid since the assumed local smoothness of μ at the interior point $\boldsymbol{z}$ ensures adequate regularity of $\boldsymbol{P}$ in a neighborhood of $\boldsymbol{z}$). The resulting leading $O(a)$ order contribution to the VIE (25) is the integral equation

$$\big(\mathcal{I} + \mathcal{L}_\infty\big)\boldsymbol{P}_1'(\bar{\boldsymbol{x}}) \;=\; \bar{\boldsymbol{x}}\cdot\big(\boldsymbol{\nabla}\boldsymbol{P} + \boldsymbol{I}\big)(\boldsymbol{z}), \qquad \bar{\boldsymbol{x}} \in \mathcal{B}, \tag{28}$$

with $\boldsymbol{P}_1'(\bar{\boldsymbol{x}}) := \boldsymbol{P}_1(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{x}}$ and the integral operator $\mathcal{L}_\infty$ defined by

$$\mathcal{L}_\infty f(\bar{\boldsymbol{x}}) = \Delta\mu \int_{\mathcal{B}} \boldsymbol{\nabla} G_\infty\big(\bar{\boldsymbol{y}} - \bar{\boldsymbol{x}}; \mu(\boldsymbol{z})\big)\cdot\boldsymbol{\nabla} f(\bar{\boldsymbol{y}})\, \mathrm{d}V(\bar{\boldsymbol{y}}). \tag{29}$$

To obtain (28), we have in particular used that

$$\Delta\boldsymbol{F}_a(G(\cdot, \boldsymbol{x})) = \Delta\mu \int_{B_a} \boldsymbol{\nabla}_1 G(\boldsymbol{y}, \boldsymbol{x})\, \mathrm{d}V(\boldsymbol{y}) = a\,[\mathcal{L}_\infty \bar{\boldsymbol{y}}](\bar{\boldsymbol{x}}) + o(a).$$

Then, letting $\boldsymbol{U}$ denote the solution of the integral equation

$$\big(\mathcal{I} + \mathcal{L}_\infty\big)\boldsymbol{U}(\bar{\boldsymbol{x}}) \;=\; \bar{\boldsymbol{x}}, \qquad \bar{\boldsymbol{x}} \in \mathcal{B}, \tag{30}$$

we have $\boldsymbol{P}_1'(\bar{\boldsymbol{x}}) = \boldsymbol{U}(\bar{\boldsymbol{x}})\cdot\big(\boldsymbol{\nabla}\boldsymbol{P} + \boldsymbol{I}\big)(\boldsymbol{z})$. The ansatz (26) therefore results in the inner expansion

$$\boldsymbol{P}_a(\boldsymbol{x}) = \boldsymbol{P}(\boldsymbol{z}) + a\big\{\boldsymbol{U}(\bar{\boldsymbol{x}})\cdot\big(\boldsymbol{\nabla}\boldsymbol{P} + \boldsymbol{I}\big)(\boldsymbol{z}) - \bar{\boldsymbol{x}}\big\} + o(a), \qquad \boldsymbol{x} \in B_a,\ \bar{\boldsymbol{x}} \in \mathcal{B} \tag{31}$$

of $\boldsymbol{P}_a$, whose justification then stems from the following lemma (whose proof is given in Appendix A).

LEMMA 2. *There exists a constant $a_P > 0$ such that*

$$\big\|\boldsymbol{P}_a(\boldsymbol{x}) - \boldsymbol{P}(\boldsymbol{z}) - a\big\{\boldsymbol{U}(\bar{\boldsymbol{x}})\cdot\big(\boldsymbol{\nabla}\boldsymbol{P} + \boldsymbol{I}\big)(\boldsymbol{z}) - \bar{\boldsymbol{x}}\big\}\big\|_{H^1(B_a)} = O(a^2), \qquad a < a_P. \tag{32}$$

The perturbation $\boldsymbol{p}_a$ also obeys the following lemma, given for later reference and proved in Appendix B.

LEMMA 3. *The perturbation $\boldsymbol{p}_a = \boldsymbol{P}_a - \boldsymbol{P}$ satisfies $\|\boldsymbol{p}_a\|_{L^2(Y)} = o(a)$.*

3.2. Cell solution asymptotics: The main result. The second and third cell problems (17b) and (17c) can likewise be reformulated as VIEs, rendering the asymptotic treatment of their inner solutions amenable to the same general approach. Unlike (25), however, the right-hand sides of the governing VIEs for $\boldsymbol{Q}_a$ and $\boldsymbol{R}_a$ feature integrals over Y in addition to those over B_a. This makes the derivation of their leading-order asymptotic form more involved, and the corresponding proofs are deferred to section 5. The asymptotic form (31) of $\boldsymbol{P}_a$ and the analogous results established in section 5 for $\boldsymbol{Q}_a$ and $\boldsymbol{R}_a$ are gathered in the following proposition.

PROPOSITION 4. *The cell functions $\boldsymbol{P}_a, \boldsymbol{Q}_a, \boldsymbol{R}_a$ admit in B_a the following expansions:*

$$\begin{aligned}
\boldsymbol{P}_a(\boldsymbol{x}) &= \boldsymbol{P}(\boldsymbol{z}) + a\big\{\boldsymbol{U}(\bar{\boldsymbol{x}})\cdot\big(\boldsymbol{\nabla}\boldsymbol{P}+\boldsymbol{I}\big)(\boldsymbol{z}) - \bar{\boldsymbol{x}}\big\} \,+\, o(a),\\
\boldsymbol{Q}_a(\boldsymbol{x}) &= \boldsymbol{Q}(\boldsymbol{z}) + a\big\{\boldsymbol{U}(\bar{\boldsymbol{x}})\cdot\big(\boldsymbol{\nabla}\boldsymbol{Q}+\boldsymbol{I}\otimes\boldsymbol{P}\big)(\boldsymbol{z}) - \bar{\boldsymbol{x}}\otimes\boldsymbol{P}(\boldsymbol{z})\big\} \,+\, o(a),\\
&\qquad \boldsymbol{x}\in B_a,\ \bar{\boldsymbol{x}} := a^{-1}(\boldsymbol{x}-\boldsymbol{z})\in\mathcal{B},\\
\boldsymbol{R}_a(\boldsymbol{x}) &= \boldsymbol{R}(\boldsymbol{z}) + a\big\{\boldsymbol{U}(\bar{\boldsymbol{x}})\cdot\big(\boldsymbol{\nabla}\boldsymbol{R}+\boldsymbol{I}\otimes\boldsymbol{Q}\big)(\boldsymbol{z}) - \bar{\boldsymbol{x}}\otimes\boldsymbol{Q}(\boldsymbol{z})\big\} \,+\, o(a),
\end{aligned}$$

where $\boldsymbol{U}$ is the solution of the canonic integral equation (30).

Remark 1. The VIE (30) is identical to that arising for an inhomogeneity $\mathcal{B}$ (with modulus $\mu(\boldsymbol{z})+\Delta\mu$) embedded in a homogeneous background $\mathbb{R}^2$ with modulus $\mu(\boldsymbol{z})$, subjected to a uniform far-field gradient.

3.3. Polarization tensor and expansion of integrals. In the following, we will repeatedly use expansions of quantities such as $\big\langle\!\big\langle \boldsymbol{w}, \boldsymbol{P}_a\big\rangle\!\big\rangle_{B_a}^{\Delta\mu}$, where the (possibly tensor-valued) function $\boldsymbol{w}$ is regular in a neighborhood of B_a and does not depend on a. Thanks to Proposition 4 and the Taylor expansion of $\boldsymbol{w}$ about $\boldsymbol{z}$, we have

$$\begin{aligned}
&\big\langle\!\big\langle \boldsymbol{w}, \boldsymbol{P}_a\big\rangle\!\big\rangle_{B_a}^{\Delta\mu}\\
&\quad= \Delta\mu\int_{B_a}(\boldsymbol{\nabla}\boldsymbol{w})^{\mathrm{T}}\cdot\boldsymbol{\nabla}\boldsymbol{P}_a\,\mathrm{d}V\\
&\quad= a^2\Delta\mu(\boldsymbol{\nabla}\boldsymbol{w})^{\mathrm{T}}(\boldsymbol{z})\cdot\Big\{\int_{\mathcal{B}}\boldsymbol{\nabla}\boldsymbol{U}(\bar{\boldsymbol{y}})\cdot\big(\boldsymbol{\nabla}\boldsymbol{P}+\boldsymbol{I}\big)(\boldsymbol{z})\,\mathrm{d}V(\bar{\boldsymbol{y}}) - |\mathcal{B}|\boldsymbol{I}\Big\} + o(a^2).
\end{aligned}$$

We introduce the polarization tensor $\boldsymbol{A}$ given by

$$\boldsymbol{A} = \boldsymbol{A}(\mathcal{B},\mu(\boldsymbol{z}),\Delta\mu) \;:=\; \Delta\mu\int_{\mathcal{B}}\boldsymbol{\nabla}\boldsymbol{U}(\bar{\boldsymbol{y}})\,\mathrm{d}V(\bar{\boldsymbol{y}}), \tag{34}$$

this definition being identical to that used in many earlier asymptotic studies involving nonperiodic media, e.g., [10, 15, 1]. The tensor $\boldsymbol{A}$ is, in particular known to be symmetric (e.g., [10, Lemma 5]). The above expansion of $\big\langle\!\big\langle \boldsymbol{w}, \boldsymbol{P}_a\big\rangle\!\big\rangle_{B_a}^{\Delta\mu}$ then takes the more concise form

$$\big\langle\!\big\langle \boldsymbol{w}, \boldsymbol{P}_a\big\rangle\!\big\rangle_{B_a}^{\Delta\mu} = a^2(\boldsymbol{\nabla}\boldsymbol{w})^{\mathrm{T}}(\boldsymbol{z})\cdot\big\{\boldsymbol{A}\cdot\big(\boldsymbol{\nabla}\boldsymbol{P}+\boldsymbol{I}\big) - \Delta\mu|\mathcal{B}|\boldsymbol{I}\big\}(\boldsymbol{z}) + o(a^2). \tag{35}$$

Similar expansions involving $\boldsymbol{Q}_a$ and $\boldsymbol{R}_a$ are obtained, using Proposition 4 and (34), as

$$\big\langle\!\big\langle \boldsymbol{w}, \boldsymbol{Q}_a\big\rangle\!\big\rangle_{B_a}^{\Delta\mu} = a^2(\boldsymbol{\nabla}\boldsymbol{w})^{\mathrm{T}}(\boldsymbol{z})\cdot\big\{\boldsymbol{A}\cdot\big(\boldsymbol{\nabla}\boldsymbol{Q}+\boldsymbol{I}\otimes\boldsymbol{P}\big) - \Delta\mu|\mathcal{B}|\boldsymbol{I}\otimes\boldsymbol{P}\big\}(\boldsymbol{z}) + o(a^2), \tag{36a}$$

$$\big\langle\!\big\langle \boldsymbol{w}, \boldsymbol{R}_a\big\rangle\!\big\rangle_{B_a}^{\Delta\mu} = a^2(\boldsymbol{\nabla}\boldsymbol{w})^{\mathrm{T}}(\boldsymbol{z})\cdot\big\{\boldsymbol{A}\cdot\big(\boldsymbol{\nabla}\boldsymbol{R}+\boldsymbol{I}\otimes\boldsymbol{Q}\big) - \Delta\mu|\mathcal{B}|\boldsymbol{I}\otimes\boldsymbol{Q}\big\}(\boldsymbol{z}) + o(a^2). \tag{36b}$$

4. Topological sensitivities. The following theorem, whose proof is deferred to section 6, gives the TSs of the effective material properties featured in the field equation (16) governing the third-order approximation of the mean (macroscopic) wavefield in a medium with periodic microstructure; it is the main result of this work.

THEOREM 5. *Consider a small inhomogeneity $B_a = \boldsymbol{z} + a\mathcal{B}$ with radius a, shape $\mathcal{B}$, shear modulus $\mu + \Delta\mu$, and mass density $\rho + \Delta\rho$ (where $\Delta\mu > -\min_{\boldsymbol{x}\in Y} \mu(\boldsymbol{x})$ and $\Delta\rho > -\min_{\boldsymbol{x}\in Y} \rho(\boldsymbol{x})$ are uniform material contrasts), nucleated at some point $\boldsymbol{z} \in Y$ inside the periodic unit cell. Moreover, let the adjoint solutions $\beta \in \mathcal{V}$ and (for any $\boldsymbol{v} \in \boldsymbol{\mathcal{V}}_p$) $\boldsymbol{X}[\boldsymbol{v}] \in \boldsymbol{\mathcal{V}}_{p+1}$ be defined by problems*

$$\text{(37a)} \qquad \langle\!\langle w, \beta \rangle\!\rangle_Y^{\mu} = \int_Y (\rho - \varrho^0) w \, dV \qquad \text{for all } w \in \mathcal{V},$$

$$\text{(37b)} \qquad \langle\!\langle w, \boldsymbol{X}[\boldsymbol{v}] \rangle\!\rangle_Y^{\mu} = \boldsymbol{J}(\boldsymbol{v}, w) \qquad \text{for all } w \in \mathcal{V}.$$

The affiliated TSs of the effective material properties (6) *and* (8)*, as defined through expansion* (20) *with $\upsilon(a) = |Y|^{-1}a^2$, are given in terms of the background cell functions $\boldsymbol{P}, \boldsymbol{Q}, \boldsymbol{R}$, the adjoint solutions β and $\boldsymbol{X}[\beta]$, and the polarization tensor $\boldsymbol{A}$ by*

$$\begin{aligned}
\mathcal{D}\varrho^0(\boldsymbol{z}) &= |\mathcal{B}|\Delta\rho,\\
\mathcal{D}\boldsymbol{\mu}^0(\boldsymbol{z}) &= \Big\{ \big(\boldsymbol{\nabla}\boldsymbol{P} + \boldsymbol{I}\big)^T \cdot \boldsymbol{A} \cdot \big(\boldsymbol{\nabla}\boldsymbol{P} + \boldsymbol{I}\big) \Big\}(\boldsymbol{z}),\\
\mathcal{D}\boldsymbol{\varrho}^1(\boldsymbol{z}) &= \Big\{ \mathcal{D}\varrho^0 \boldsymbol{P} - \boldsymbol{\nabla}\beta \cdot \boldsymbol{A} \cdot \big(\boldsymbol{\nabla}\boldsymbol{P} + \boldsymbol{I}\big) \Big\}(\boldsymbol{z}),\\
\mathcal{D}\boldsymbol{\mu}^1(\boldsymbol{z}) &= \frac{1}{\varrho^0} \Big\{ \mathcal{D}\boldsymbol{\varrho}^1 \otimes \boldsymbol{\mu}^0 + \boldsymbol{\varrho}^1 \otimes \mathcal{D}\boldsymbol{\mu}^0 - \mathcal{D}\varrho^0 \boldsymbol{\varrho}^1 \otimes \frac{\boldsymbol{\mu}^0}{\varrho^0} \Big\}_{\text{sym}}(\boldsymbol{z}),\\
\mathcal{D}\boldsymbol{\varrho}^2(\boldsymbol{z}) &= \Big\{ \big(-\boldsymbol{\nabla}\boldsymbol{X}[\beta] + \beta\boldsymbol{I}\big) \cdot \boldsymbol{A} \cdot \big(\boldsymbol{\nabla}\boldsymbol{P} + \boldsymbol{I}\big) - \boldsymbol{\nabla}\beta \cdot \boldsymbol{A} \cdot \big(\boldsymbol{\nabla}\boldsymbol{Q} + \boldsymbol{I} \otimes \boldsymbol{P}\big) \Big\}_{\text{sym}}(\boldsymbol{z})\\
&\quad + \Big\{ \mathcal{D}\varrho^0 \Big(\boldsymbol{Q} - \beta \frac{\boldsymbol{\mu}^0}{\varrho^0} \Big) - \frac{\langle \rho\beta \rangle}{\varrho^0} \Big(\mathcal{D}\boldsymbol{\mu}^0 - \mathcal{D}\varrho^0 \frac{\boldsymbol{\mu}^0}{\varrho^0} \Big) \Big\}_{\text{sym}}(\boldsymbol{z}),\\
\mathcal{D}\boldsymbol{\mu}^2(\boldsymbol{z}) &= \Big\{ 2\big(\boldsymbol{\nabla}\boldsymbol{P} + \boldsymbol{I}\big)^T \cdot \boldsymbol{A} \cdot \big(\boldsymbol{\nabla}\boldsymbol{R} + \boldsymbol{I} \otimes \boldsymbol{Q}\big)\\
&\qquad - \big(\boldsymbol{\nabla}\boldsymbol{Q} + \boldsymbol{I} \otimes \boldsymbol{P}\big)^T \cdot \boldsymbol{A} \cdot \big(\boldsymbol{\nabla}\boldsymbol{Q} + \boldsymbol{I} \otimes \boldsymbol{P}\big) \Big\}_{\text{sym}}(\boldsymbol{z})\\
&\quad + \Big\{ \big[\mathcal{D}\boldsymbol{\varrho}^2 + \mathcal{D}\varrho^0 \big(\boldsymbol{P} \otimes \boldsymbol{P} - 2\boldsymbol{Q} \big) \big] \otimes \frac{\boldsymbol{\mu}^0}{\varrho^0} + \frac{1}{\varrho^0} \big(\langle \rho \boldsymbol{P} \otimes \boldsymbol{P} \rangle - \boldsymbol{\varrho}^2 \big)\\
&\qquad \otimes \Big(\mathcal{D}\boldsymbol{\mu}^0 - \mathcal{D}\varrho^0 \frac{\boldsymbol{\mu}^0}{\varrho^0} \Big) \Big\}_{\text{sym}}(\boldsymbol{z}).
\end{aligned}$$

Remark 2. Lemma 1, which holds true for any configuration of the material in Y, implies that $\mathcal{D}\varrho^0$, $\mathcal{D}\boldsymbol{\varrho}^1$, $\mathcal{D}\boldsymbol{\mu}^0$, and $\mathcal{D}\boldsymbol{\mu}^1$ are related through

$$\{\mathcal{D}\boldsymbol{\varrho}^1 \otimes \boldsymbol{\mu}^0 + \boldsymbol{\varrho}^1 \otimes \mathcal{D}\boldsymbol{\mu}^0\}_{\text{sym}} = \mathcal{D}\varrho^0 \boldsymbol{\mu}^1 + \varrho^0 \mathcal{D}\boldsymbol{\mu}^1.$$

Indeed, expressing $\mathcal{D}\boldsymbol{\mu}^1$ by means of this identity yields the formula given in Theorem 5.

Remark 3. Consider the case where the background material parameters μ, ρ are only piecewise smooth. Then, transmission conditions of the form $[\![\boldsymbol{v}]\!] = \boldsymbol{0}$ and $[\![\mu\, \boldsymbol{n} \cdot \boldsymbol{\nabla}\boldsymbol{v}]\!] = \boldsymbol{0}$ must be added [27] to the cell problems in strong form (with

$\boldsymbol{v} = \boldsymbol{P}, \boldsymbol{Q}, \boldsymbol{R}$ for problems (5) and $\boldsymbol{v} = G(\cdot, \boldsymbol{x})$ for problem (21)), and are implicitly embedded in the weak problem (11). The TS formulas given by Theorem 5 remain valid in this case, provided the inhomogeneity locus $\boldsymbol{z}$ lies away from any material discontinuity line. This stems from the fact that the analyses carried out in sections 3 and 4 require μ and ρ to be smooth only in a neighborhood of $\boldsymbol{z}$. For example, this weakened assumption is sufficient for decomposition (22) of the Green's function to hold and for Taylor expansions of the background cell solutions to have requisite local validity wherever required.

Remark 4. In the case of constant mass density, $\varrho^0 = \rho$ while $\boldsymbol{\varrho}^1, \boldsymbol{\varrho}^2, \beta$, and $\boldsymbol{\mu}^1$ vanish identically (the latter by Lemma 1). In such situations, the dependence on $\Delta\rho$ and $\Delta\mu$ of the featured TSs occurs via the terms $\mathcal{D}\varrho^0 = |\mathcal{B}|\Delta\rho$ and $\boldsymbol{A}$, respectively. With reference to (16), the resulting formula $\mathcal{D}\boldsymbol{\varrho}^2(\boldsymbol{z}) = \left\{\mathcal{D}\varrho^0 \boldsymbol{Q}\right\}_{\mathrm{sym}}(\boldsymbol{z})$, in particular, characterizes the singular perturbation of the governing field equation once a point-like inertial heterogeneity is periodically introduced in a medium with otherwise constant mass density. In the context of the second-order macroscopic model for waves in periodic media, this perturbation $(\omega^2\boldsymbol{\varrho}^2 : \boldsymbol{\nabla}^2(\cdot))$ is solely responsible for the coupling between the temporal and spatial derivatives.

In the case of constant shear modulus, we have $\boldsymbol{P} = \boldsymbol{0}$ by the well-posedness of the homogeneous problem (5a), implying $\boldsymbol{\mu}^0 = \mu\boldsymbol{I}$ and $\boldsymbol{\varrho}^1 = \boldsymbol{0}$, as well as $\mathcal{D}\boldsymbol{\mu}^0 = \boldsymbol{A}$ (as shown by [2]).

Remark 5. If B_a is an ellipse such that $\mathcal{B}$ has principal directions $(\boldsymbol{a}_1, \boldsymbol{a}_2)$ and semiaxes lengths $(1, \gamma)$, we have [1]

$$|\mathcal{B}| = \pi\gamma, \quad \boldsymbol{A} = \pi\gamma(\gamma+1)\mu(\boldsymbol{z}) \left[\frac{\kappa(\boldsymbol{z})}{1+\gamma+\gamma\kappa(\boldsymbol{z})}\boldsymbol{a}_1\otimes\boldsymbol{a}_1 + \frac{\kappa(\boldsymbol{z})}{1+\gamma+\kappa(\boldsymbol{z})}\boldsymbol{a}_2\otimes\boldsymbol{a}_2\right], \tag{38}$$

having set $\kappa(\boldsymbol{z}) := \Delta\mu/\mu(\boldsymbol{z})$. The case where B_a is a disk corresponds to $\gamma = 1$.

Remark 6. The present expression for the TS $\mathcal{D}\boldsymbol{\mu}^0$ has the same structure as that given by [14] for plane-strain two-dimensional elastostatics.

5. Cell solution asymptotics: Proofs for the second and third problems. Following the approach of section 3.1, the unperturbed cell functions $\boldsymbol{Q}$ and $\boldsymbol{R}$ are found to read

$$\boldsymbol{Q}(\boldsymbol{x}) = \boldsymbol{J}(G(\cdot, \boldsymbol{x}), \boldsymbol{P}) + \boldsymbol{K}^Q(G(\cdot, \boldsymbol{x})) - \boldsymbol{L}^Q(G(\cdot, \boldsymbol{x})), \tag{39a}$$

$$\boldsymbol{R}(\boldsymbol{x}) = \boldsymbol{J}(G(\cdot, \boldsymbol{x}), \boldsymbol{Q}) + \boldsymbol{K}^R(G(\cdot, \boldsymbol{x})) - \boldsymbol{L}^R(G(\cdot, \boldsymbol{x})), \tag{39b}$$

where G is the periodic Green's function given by (21). The relevant weak problems (11b), (11c), (17b), and (17c) for the perturbed cell then help demonstrate that the restrictions of $\boldsymbol{Q}_a$ and $\boldsymbol{R}_a$ to B_a satisfy the VIEs

$$\begin{aligned}(\mathcal{I}+\mathcal{L}_a)\boldsymbol{Q}_a(\boldsymbol{x}) &= \boldsymbol{Q}(\boldsymbol{x}) + \Delta\boldsymbol{J}_a(G(\cdot, \boldsymbol{x}), \boldsymbol{P}_a) + \boldsymbol{J}(G(\cdot, \boldsymbol{x}), \boldsymbol{p}_a) + \Delta\boldsymbol{K}_a^Q(G(\cdot, \boldsymbol{x})) \\ &\quad - \Delta\boldsymbol{L}_a^Q(G(\cdot, \boldsymbol{x})),\end{aligned} \tag{40a}$$

$$\begin{aligned}(\mathcal{I}+\mathcal{L}_a)\boldsymbol{R}_a(\boldsymbol{x}) &= \boldsymbol{R}(\boldsymbol{x}) + \Delta\boldsymbol{J}_a(G(\cdot, \boldsymbol{x}), \boldsymbol{Q}_a) + \boldsymbol{J}(G(\cdot, \boldsymbol{x}), \boldsymbol{q}_a) + \Delta\boldsymbol{K}_a^R(G(\cdot, \boldsymbol{x})) \\ &\quad - \Delta\boldsymbol{L}_a^R(G(\cdot, \boldsymbol{x})).\end{aligned} \tag{40b}$$

5.1. Second cell problem. Consider an inner expansion of the second cell solution $\boldsymbol{Q}_a$ of the form

$$\boldsymbol{Q}_a(\boldsymbol{x}) \;=\; \boldsymbol{Q}(\boldsymbol{z}) + a\boldsymbol{Q}_1(\bar{\boldsymbol{x}}) + o(a).$$

The corresponding expansion of VIE (40a) follows the same general approach as that of (25), but is more involved as it requires determining the asymptotic behavior of various terms appearing on the right-hand side of (40a).

Asymptotic form of $\boldsymbol{\Delta K_a^Q(G(\cdot,x))}$ and $\boldsymbol{\Delta L_a^Q(G(\cdot,x))}$. Both $\Delta\boldsymbol{K}_a^Q(G(\cdot,\boldsymbol{x}))$ and $\Delta\boldsymbol{L}_a^Q(G(\cdot,\boldsymbol{x}))$ are integrals over B_a that involve G but not its gradient. On recalling the definitions (13) of $\boldsymbol{K}_a^Q$ and $\boldsymbol{L}_a^Q$, introducing the scaled coordinates in the relevant integrals, and invoking the asymptotic behavior (27a) of G, one finds via (27a) that

$$\Delta\boldsymbol{K}_a^Q(G(\cdot,\boldsymbol{x})) = O(a^2\ln a), \qquad \Delta\boldsymbol{L}_a^Q(G(\cdot,\boldsymbol{x})) = O(a^2\ln a). \tag{41a}$$

Asymptotic form of $\boldsymbol{\Delta J_a(G(\cdot,x),P_a)}$. From definition (12), we have

$$\begin{aligned}\Delta\boldsymbol{J}_a(G(\cdot,\boldsymbol{x}),\boldsymbol{P}_a) = \Delta\mu\int_{B_a} G(\boldsymbol{y},\boldsymbol{x})\boldsymbol{\nabla}\boldsymbol{P}_a(\boldsymbol{y})\,\mathrm{d}V(\boldsymbol{y})\\ -\Delta\mu\int_{B_a}\boldsymbol{\nabla}_1 G(\boldsymbol{y},\boldsymbol{x})\otimes\boldsymbol{P}_a(\boldsymbol{y})\,\mathrm{d}V(\boldsymbol{y}), \qquad \boldsymbol{x}\in B_a.\end{aligned}$$

For $\boldsymbol{y},\boldsymbol{x}\in B_a$, one has $G(\boldsymbol{y},\boldsymbol{x}) = O(\ln a)$, $\boldsymbol{\nabla}\boldsymbol{P}_a(\boldsymbol{y}) = O(1)$ thanks to (31), and $\mathrm{d}V(\boldsymbol{y}) = O(a^2)$. Accordingly, the first integral above behaves as $O(a^2\ln a)$. On the other hand, from (27b) and (31), one finds the the second integral to be $O(a)$, and we have

$$\begin{aligned}\Delta\boldsymbol{J}_a(G(\cdot,\boldsymbol{x}),\boldsymbol{P}_a) &= -a\Big\{\Delta\mu\int_{\mathcal{B}}\boldsymbol{\nabla}G_\infty(\bar{\boldsymbol{y}}-\bar{\boldsymbol{x}};\mu(\boldsymbol{z}))\,\mathrm{d}V(\bar{\boldsymbol{y}})\Big\}\otimes\boldsymbol{P}_a(\boldsymbol{z}) \;+\; o(a)\\ &= -a\,\mathcal{L}_\infty\big[\bar{\boldsymbol{y}}\otimes\boldsymbol{P}(\boldsymbol{z})\big](\bar{\boldsymbol{x}}) \;+\; o(a), \qquad \boldsymbol{x}\in B_a.\end{aligned} \tag{41b}$$

Asymptotic form of $\boldsymbol{J(G(\cdot,x),p_a)}$. Recalling (12), this term is defined as an integral over the whole cell Y, which makes its asymptotic evaluation as $a\to 0$ less straightforward (see also Remark 7 below). We circumvent this difficulty by an indirect evaluation of $\boldsymbol{J}(G(\cdot,\boldsymbol{x}),\boldsymbol{p}_a)$. Let $\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]$ be the solution of the adjoint problem (37b) with $\boldsymbol{v} = G(\cdot,\boldsymbol{x})$, i.e.,

$$\big\langle\!\big\langle w,\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]\big\rangle\!\big\rangle_Y^\mu \;=\; \boldsymbol{J}(G(\cdot,\boldsymbol{x}),w) \qquad \text{for all } w\in\mathcal{V}.$$

By definition (12), $\boldsymbol{J}(G(\cdot,\boldsymbol{x}),w)$ is a combination of volume potentials (with densities w and $\boldsymbol{\nabla}w$), whose known mapping properties (see, e.g., [17, Thm. 6.1.12]) ensure that $w\mapsto\boldsymbol{J}(G(\cdot,\boldsymbol{x}),w)$ is a continuous linear functional on $H^1(Y)$. Therefore, the variational problem (41) is well-posed. On setting $w=\boldsymbol{p}_a$, we accordingly have

$$\boldsymbol{J}(G(\cdot,\boldsymbol{x}),\boldsymbol{p}_a) = \big\langle\!\big\langle\boldsymbol{p}_a,\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]\big\rangle\!\big\rangle_Y^\mu = \big(\big\langle\!\big\langle\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big],\boldsymbol{p}_a\big\rangle\!\big\rangle_Y^\mu\big)^{\mathrm{T}}. \tag{41c}$$

Next, we use the weak formulation (18a) for $\boldsymbol{p}_a$ with $w=\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]$, which allows us to express $\boldsymbol{J}(G(\cdot,\boldsymbol{x}),\boldsymbol{p}_a)$ in terms of integrals over the vanishing inclusion support

B_a:

$$\begin{aligned}\boldsymbol{J}(G(\cdot,\boldsymbol{x}),\boldsymbol{p}_a) &= -\Big(\big\langle\!\big\langle \boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big],\boldsymbol{P}_a\big\rangle\!\big\rangle_{B_a}^{\Delta\mu} + \Delta\boldsymbol{F}_a\big(\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]\big)\Big)^{\mathrm{T}}\\ &= -\Delta\mu\int_{B_a}(\boldsymbol{\nabla}\boldsymbol{P}_a+\boldsymbol{I})^{\mathrm{T}}\cdot\boldsymbol{\nabla}\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]\,\mathrm{d}V.\end{aligned}$$

By the Cauchy–Schwarz inequality, and since the first cell solution asymptotics (31) allows one to show that $\|\boldsymbol{\nabla}\boldsymbol{P}_a+\boldsymbol{I}\|_{L^2(B_a)}\leqslant Ca$ for some $C>0$, we have

$$\begin{aligned}\big|\boldsymbol{J}(G(\cdot,\boldsymbol{x}),\boldsymbol{p}_a)\big| &\leqslant |\Delta\mu|\big\|\boldsymbol{\nabla}\boldsymbol{P}_a+\boldsymbol{I}\big\|_{L^2(B_a)}\big\|\boldsymbol{\nabla}\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]\big\|_{L^2(B_a)}\\ &\leqslant Ca|\Delta\mu|\big\|\boldsymbol{\nabla}\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]\big\|_{L^2(B_a)}.\end{aligned}$$

Moreover, since $\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]$ is an $H^1(Y)$ function that does not depend on a, $\big|\boldsymbol{\nabla}\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]\big|^2\chi_{B_a}$ defines a sequence of measurable functions whose pointwise limit is zero almost everywhere in Y. Consequently, $\big\|\boldsymbol{\nabla}\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]\big\|_{L^2(B_a)}\to 0$ as $a\to 0$ by Lebesgue's dominated convergence theorem, and we obtain

$$\boldsymbol{J}(G(\cdot,\boldsymbol{x}),\boldsymbol{p}_a)=o(a). \tag{41d}$$

Remark 7. Merely using that the mapping $w\mapsto\boldsymbol{J}(G(\cdot,\boldsymbol{x}),w)$ is continuous on $H^1(Y)$ together with the known estimate $\|\boldsymbol{p}_a\|_{H^1(Y)}=O(a)$ would only yield the suboptimal estimate $\boldsymbol{J}(G(\cdot,\boldsymbol{x}),\boldsymbol{p}_a)=O(a)$.

Inner expansion of $\boldsymbol{Q}_a$. By virtue of (41a), (41b), (41d), one finds the leading-order ($O(a)$) behavior of the VIE (40a) to read

$$\big(\mathcal{I}+\mathcal{L}_\infty\big)\boldsymbol{Q}_1'(\bar{\boldsymbol{x}}) \;=\; \bar{\boldsymbol{x}}\cdot\big(\boldsymbol{\nabla}\boldsymbol{Q}+\boldsymbol{I}\otimes\boldsymbol{P}\big)(\boldsymbol{z}),$$

having set $\boldsymbol{Q}_1'(\bar{\boldsymbol{x}}):=\boldsymbol{Q}_1(\bar{\boldsymbol{x}})+\bar{\boldsymbol{x}}\otimes\boldsymbol{P}(\boldsymbol{z})$. The inner expansion of $\boldsymbol{Q}_a$ is therefore given by

$$\boldsymbol{Q}_a(\boldsymbol{x})=\boldsymbol{Q}(\boldsymbol{z})+a\big\{\boldsymbol{U}(\bar{\boldsymbol{x}})\cdot\big(\boldsymbol{\nabla}\boldsymbol{Q}+\boldsymbol{I}\otimes\boldsymbol{P}\big)(\boldsymbol{z})-\bar{\boldsymbol{x}}\otimes\boldsymbol{P}(\boldsymbol{z})\big\}+o(a),\quad \boldsymbol{x}\in B_a,\ \bar{\boldsymbol{x}}\in\mathcal{B}, \tag{42}$$

where $\boldsymbol{U}$ again solves (30).

5.2. Third cell problem. Following the same approach, we seek the inner expansion of the third cell solution as

$$\boldsymbol{R}_a(\boldsymbol{x})=\boldsymbol{R}(\boldsymbol{z})+a\boldsymbol{R}_1(\bar{\boldsymbol{x}})+o(a).$$

The expansion of the VIE (40b), like that of (40a), requires determining the asymptotic behavior of various terms appearing in its right-hand side, some of them defined as integrals over Y.

Asymptotic form of $\Delta\boldsymbol{K}_a^{\boldsymbol{R}}(\boldsymbol{G}(\cdot,\boldsymbol{x}))$ and $\Delta\boldsymbol{L}_a^{\boldsymbol{R}}(\boldsymbol{G}(\cdot,\boldsymbol{x}))$. From definition (13), we have

$$\Delta\boldsymbol{K}_a^R(G(\cdot,\boldsymbol{x})) \;=\; \Delta\mu\int_{B_a}G(\cdot,\boldsymbol{x})\boldsymbol{I}\otimes\boldsymbol{P}_a\,\mathrm{d}V+\int_Y\mu G(\cdot,\boldsymbol{x})\boldsymbol{I}\otimes\boldsymbol{p}_a\,\mathrm{d}V.$$

The first term on the right-hand side behaves as $O(a^2\ln a)$ by the argument used to obtain (41a). Moreover, Lemma 3 and the Cauchy–Schwartz inequality ($G(\cdot,\boldsymbol{x})$ being

a $L^2(Y)$ function) imply that the second integral behaves as $o(a)$. A similar analysis applies to $\Delta \boldsymbol{L}_a^R(G(\cdot,\boldsymbol{x}))$, given by

$$\Delta \boldsymbol{L}_a^R(G(\cdot,\boldsymbol{x})) = \Delta\rho \int_{B_a} G(\cdot,\boldsymbol{x}) \frac{\boldsymbol{\mu}_a^0}{\varrho_a^0} \otimes \boldsymbol{P}_a \,\mathrm{d}V + \int_Y \rho G(\cdot,\boldsymbol{x}) \Big\{ \Big(\frac{\boldsymbol{\mu}_a^0}{\varrho_a^0} - \frac{\boldsymbol{\mu}^0}{\varrho^0} \Big) \otimes \boldsymbol{P}_a + \frac{\boldsymbol{\mu}^0}{\varrho^0} \otimes \boldsymbol{p}_a \Big\} \,\mathrm{d}V,$$

using, in addition, the fact that $\boldsymbol{\mu}_a^0/\varrho_a^0 - \boldsymbol{\mu}^0/\varrho^0 = O(\upsilon(a)) = O(a^2)$ by Theorem 5 (this invocation being legitimate since that part of Theorem 5 only relies on the asymptotic behavior of $\boldsymbol{P}_a$). Concluding, we have

$$\Delta \boldsymbol{K}_a^R(G(\cdot,\boldsymbol{x})) = o(a), \qquad \Delta \boldsymbol{L}_a^R(G(\cdot,\boldsymbol{x})) = o(a). \tag{43a}$$

Asymptotic form of $\Delta \boldsymbol{J}_a(G(\cdot,\boldsymbol{x}),\boldsymbol{Q}_a)$. A derivation analogous to that of (41b) gives

$$\begin{aligned} \Delta \boldsymbol{J}_a(G(\cdot,\boldsymbol{x}),\boldsymbol{Q}_a) &= -a \Big\{ \Delta\mu \int_{\mathcal{B}} \boldsymbol{\nabla} G_\infty(\bar{\boldsymbol{y}} - \bar{\boldsymbol{x}}; \mu(\boldsymbol{z}))\, \mathrm{d}V(\bar{\boldsymbol{y}}) \Big\} \otimes \boldsymbol{Q}_a(\boldsymbol{z}) + o(a) \\ &= -a \mathcal{L}_\infty \big[\bar{\boldsymbol{y}} \otimes \boldsymbol{Q}(\boldsymbol{z}) \big](\bar{\boldsymbol{x}}) + o(a), \qquad \boldsymbol{x} \in B_a. \end{aligned} \tag{43b}$$

Asymptotic form of $\boldsymbol{J}(\boldsymbol{G}(\cdot,\boldsymbol{x}),\boldsymbol{q}_a)$. By analogy to the case of $\boldsymbol{J}(G(\cdot,\boldsymbol{x}),\boldsymbol{p}_a)$, the term $\boldsymbol{J}(G(\cdot,\boldsymbol{x}),\boldsymbol{q}_a)$—given by an integral over the whole cell Y—can be recast as

$$\boldsymbol{J}(G(\cdot,\boldsymbol{x}),\boldsymbol{q}_a) \;=\; \big\langle\!\!\big\langle \boldsymbol{q}_a, \boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big] \big\rangle\!\!\big\rangle_Y^\mu \;=\; \big(\big\langle\!\!\big\langle \boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big], \boldsymbol{q}_a \big\rangle\!\!\big\rangle_Y^\mu \big)^{\mathrm{T}}.$$

Then, invoking problem (18b) with $\boldsymbol{w} = \boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]$, we obtain

$$\begin{aligned} \big\langle\!\!\big\langle \boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big], \boldsymbol{q}_a \big\rangle\!\!\big\rangle_Y^\mu &= -\big\langle\!\!\big\langle \boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big], \boldsymbol{Q}_a \big\rangle\!\!\big\rangle_{B_a}^{\Delta\mu} + \Delta \boldsymbol{J}_a(\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big], \boldsymbol{P}_a) \\ &\quad + \boldsymbol{J}(\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big], \boldsymbol{p}_a) + \Delta \boldsymbol{K}_a^Q(\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]) - \Delta \boldsymbol{L}_a^Q(\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big]). \end{aligned} \tag{43c}$$

Thanks to (41c), we have

$$\boldsymbol{J}(\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big], \boldsymbol{p}_a) = \big(\big\langle\!\!\big\langle \boldsymbol{X}\big[\boldsymbol{X}[G(\cdot,\boldsymbol{x})]\big], \boldsymbol{p}_a \big\rangle\!\!\big\rangle_Y^\mu \big)^{\mathrm{T}}.$$

Since $\boldsymbol{X}\big[\boldsymbol{X}[G(\cdot,\boldsymbol{x})]\big]$ is an $H^1(Y)$ function (actually having more regularity than $\boldsymbol{X}[G(\cdot,\boldsymbol{x})]$), the argument leading to (41d) applies, allowing us to show that $\boldsymbol{J}(\boldsymbol{X}\big[G(\cdot,\boldsymbol{x})\big], \boldsymbol{p}_a) = o(a)$. The remaining contributions to the right-hand side of (43c) can likewise be shown to behave as $o(a)$ thanks to (43a) and a similar argument applied to the first two terms. As a result, we have

$$\boldsymbol{J}(G(\cdot,\boldsymbol{x}),\boldsymbol{q}_a) = o(a). \tag{43d}$$

Inner expansion of $\boldsymbol{R}_a$. The VIE (40b) can now be expanded with the help of (43a), (43b), (43d). Its leading-order ($O(a)$) contribution furnishes the integral equation

$$\big(\mathcal{I} + \mathcal{L}_\infty\big) \boldsymbol{R}_1'(\bar{\boldsymbol{x}}) = \bar{\boldsymbol{x}} \cdot \big(\boldsymbol{\nabla} \boldsymbol{R} + \boldsymbol{I} \otimes \boldsymbol{Q} \big)(\boldsymbol{z}),$$

wherein $\boldsymbol{R}_1'(\bar{\boldsymbol{x}}) := \boldsymbol{R}_1(\bar{\boldsymbol{x}}) + \bar{\boldsymbol{x}} \otimes \boldsymbol{Q}(\boldsymbol{z})$. The inner expansion of $\boldsymbol{R}_a$ is therefore given by

$$\boldsymbol{R}_a(\boldsymbol{x}) = \boldsymbol{R}(\boldsymbol{z}) + a \big\{ \boldsymbol{U}(\bar{\boldsymbol{x}}) \cdot \big(\boldsymbol{\nabla} \boldsymbol{R} + \boldsymbol{I} \otimes \boldsymbol{Q} \big)(\boldsymbol{z}) - \bar{\boldsymbol{x}} \otimes \boldsymbol{Q}(\boldsymbol{z}) \big\} + o(a), \qquad \boldsymbol{x} \in B_a,\ \bar{\boldsymbol{x}} \in \mathcal{B}, \tag{44}$$

where $\boldsymbol{U}$ solves (30).

6. Proof of Theorem 5.

Density, zeroth order. By virtue of (6a), one immediately finds

$$\varrho_a^0 - \varrho^0 \;=\; \langle \rho_a - \rho \rangle \;=\; a^2 |Y|^{-1} |\mathcal{B}| \Delta\rho \;\;=\; \upsilon(a) \mathcal{D}\varrho^0.$$

Shear modulus, zeroth order. From the definition (15a) of $\boldsymbol{\mu}^0$, we have

$$\boldsymbol{\mu}_a^0 - \boldsymbol{\mu}^0 = |Y|^{-1} \Big(\Delta \boldsymbol{F}_a(\boldsymbol{P}_a) + \boldsymbol{F}(\boldsymbol{p}_a) + a^2 \Delta\mu |\mathcal{B}| \boldsymbol{I} \Big)^{\mathrm{T}}_{\mathrm{sym}}. \tag{45}$$

The leading contributions as $a \to 0$ of the right-hand side of the above equality are to be evaluated. We begin by noting that

$$\big(\Delta \boldsymbol{F}_a(\boldsymbol{P}_a) + a^2 \Delta\mu |\mathcal{B}| \boldsymbol{I} \big)^{\mathrm{T}} = \Delta\mu \int_{B_a} \big(\boldsymbol{I} + \boldsymbol{\nabla} \boldsymbol{P}_a \big) \, \mathrm{d}V = a^2 \boldsymbol{A} \big(\boldsymbol{\nabla} \boldsymbol{P} + \boldsymbol{I} \big)(\boldsymbol{z}) + o(a^2), \tag{46a}$$

where the last equality follows from expansion (31) and the definition (34) of $\boldsymbol{A}$. Turning to the contribution of $\boldsymbol{F}(\boldsymbol{p}_a)$, we have

$$(\boldsymbol{F}(\boldsymbol{p}_a))^{\mathrm{T}} = -\big\langle\!\!\big\langle \boldsymbol{P}, \boldsymbol{p}_a \big\rangle\!\!\big\rangle_Y^{\mu}$$

by virtue of (11a). Moreover, for any $\boldsymbol{w} \in \boldsymbol{\mathcal{V}}$ that is regular in the neighborhood of B_a, the weak problem (18a) for $\boldsymbol{p}_a$ implies

$$\big\langle\!\!\big\langle \boldsymbol{w}, \boldsymbol{p}_a \big\rangle\!\!\big\rangle_Y^{\mu} = -\big\langle\!\!\big\langle \boldsymbol{w}, \boldsymbol{P}_a \big\rangle\!\!\big\rangle_{B_a}^{\Delta\mu} - \Delta \boldsymbol{F}_a(\boldsymbol{w}) = -a^2 (\boldsymbol{\nabla} \boldsymbol{w})^{\mathrm{T}}(\boldsymbol{z}) \cdot \boldsymbol{A} \cdot \big(\boldsymbol{\nabla} \boldsymbol{P} + \boldsymbol{I} \big)(\boldsymbol{z}) + o(a^2), \tag{46b}$$

due to (35). Accordingly, by using $\boldsymbol{w} = \boldsymbol{P}$ in (46b) we find

$$(\boldsymbol{F}(\boldsymbol{p}_a))^{\mathrm{T}} = a^2 (\boldsymbol{\nabla} \boldsymbol{P})^{\mathrm{T}}(\boldsymbol{z}) \cdot \boldsymbol{A} \cdot \big(\boldsymbol{\nabla} \boldsymbol{P} + \boldsymbol{I} \big)(\boldsymbol{z}) + o(a^2). \tag{46c}$$

The sought for expression for $\mathcal{D}\boldsymbol{\mu}^0$ in Theorem 5 then follows from definition (20) of the TS and the use of (46a) and (46c) in (45).

Density, first order. To evaluate $\mathcal{D}\boldsymbol{\varrho}^1$, we deploy the definition (6b) of $\boldsymbol{\varrho}^1$ and write

$$\boldsymbol{\varrho}_a^1 - \boldsymbol{\varrho}^1 \;=\; \langle \rho_a \boldsymbol{P}_a - \rho \boldsymbol{P} \rangle \;=\; \Delta\rho \langle \chi_{B_a} \boldsymbol{P}_a \rangle \;+\; \langle \rho \boldsymbol{p}_a \rangle. \tag{47}$$

Then, using the expansion of $\boldsymbol{P}_a$ as in Proposition 4, we have

$$\Delta\rho \langle \chi_{B_a} \boldsymbol{P}_a \rangle \;=\; a^2 |Y|^{-1} |\mathcal{B}| \Delta\rho \boldsymbol{P}(\boldsymbol{z}) + o(a^2) \;=\; \upsilon(a) \mathcal{D}\varrho^0(\boldsymbol{z}) \boldsymbol{P}(\boldsymbol{z}) + o(a^2). \tag{48a}$$

Besides, on recalling (37a) with $w = \boldsymbol{p}_a$ and the fact that $\langle \boldsymbol{p}_a \rangle = \boldsymbol{0}$, one finds

$$\langle \rho \boldsymbol{p}_a \rangle = \big\langle \, (\rho - \varrho^0) \boldsymbol{p}_a \, \big\rangle = |Y|^{-1} \big\langle\!\!\big\langle \boldsymbol{p}_a, \beta \big\rangle\!\!\big\rangle_Y^{\mu},$$

which can then be evaluated using (46b) with $w = \beta$ as

$$\langle \rho \boldsymbol{p}_a \rangle = -\upsilon(a) \boldsymbol{\nabla} \beta(\boldsymbol{z}) \cdot \boldsymbol{A} \cdot \big(\boldsymbol{\nabla} \boldsymbol{P} + \boldsymbol{I} \big)(\boldsymbol{z}) + o(a^2). \tag{48b}$$

The sought for result for $\mathcal{D}\boldsymbol{\varrho}^1$ follows from using (48a) and (48b) in (47).

Shear modulus, first order. Recalling the definition (15b) of $\boldsymbol{\mu}^1$, we have

$$\boldsymbol{\mu}^1_a - \boldsymbol{\mu}^1 = |Y|^{-1}\Big\{ \Delta \boldsymbol{F}_a(\boldsymbol{Q}_a) + \Delta \boldsymbol{K}^Q_a(\boldsymbol{P}_a) + \boldsymbol{F}(\boldsymbol{q}_a) + \boldsymbol{K}^Q(\boldsymbol{p}_a) \Big\}_{\rm sym}. \tag{49}$$

First, we have

$$\begin{aligned} \Delta \boldsymbol{F}_a(\boldsymbol{Q}_a) + \Delta \boldsymbol{K}^Q_a(\boldsymbol{P}_a) &= \Delta\mu \int_{B_a} \big(\boldsymbol{\nabla} \boldsymbol{Q}_a + \boldsymbol{I}\otimes \boldsymbol{P}_a\big)^{\rm T} \,{\rm d}V \\ &= a^2 \big(\boldsymbol{\nabla}\boldsymbol{Q} + \boldsymbol{I}\otimes\boldsymbol{P}\big)^{\rm T}(\boldsymbol{z})\cdot \boldsymbol{A} \,+\, o(a^2), \end{aligned} \tag{50a}$$

where the last equality makes use of the symmetry of $\boldsymbol{A}$ and expansions (31), (34), and (42).

To determine the asymptotic contribution of $\boldsymbol{K}^Q(\boldsymbol{p}_a)$, we begin by using the weak problem (11b) with $w = \boldsymbol{p}_a$ and write

$$\boldsymbol{K}^Q(\boldsymbol{p}_a) = \big\langle\!\!\big\langle \boldsymbol{p}_a, \boldsymbol{Q}\big\rangle\!\!\big\rangle^\mu_Y - \boldsymbol{J}(\boldsymbol{p}_a,\boldsymbol{P}) + \boldsymbol{L}^Q(\boldsymbol{p}_a) = \Big\langle\!\!\Big\langle \boldsymbol{p}_a \,,\, \boldsymbol{Q} + \beta\frac{\boldsymbol{\mu}^0}{\varrho^0}\Big\rangle\!\!\Big\rangle^\mu_Y - \boldsymbol{J}(\boldsymbol{p}_a,\boldsymbol{P}),$$

where the second equality uses the adjoint problem (37a) with $w = \boldsymbol{p}_a$ and the fact that $\langle \boldsymbol{p}_a\rangle = \boldsymbol{0}$. On applying (46b) with $\boldsymbol{w} = \boldsymbol{Q} + \beta\boldsymbol{\mu}^0/\varrho^0$, we accordingly find

$$\boldsymbol{K}^Q(\boldsymbol{p}_a) = -a^2\big(\boldsymbol{\nabla}\boldsymbol{P}+\boldsymbol{I}\big)^{\rm T}(\boldsymbol{z})\cdot\boldsymbol{A}\cdot\Big(\boldsymbol{\nabla}\boldsymbol{Q} + \boldsymbol{\nabla}\beta\otimes\frac{\boldsymbol{\mu}^0}{\varrho^0}\Big)(\boldsymbol{z}) - \boldsymbol{J}(\boldsymbol{p}_a,\boldsymbol{P}) + o(a^2). \tag{50b}$$

The leading contribution of $\boldsymbol{F}(\boldsymbol{q}_a)^{\rm T}$ in (49) remains to be determined, and this requires a somewhat more involved derivation. First, the weak statement (11a) with $w = \boldsymbol{q}_a$ gives

$$\boldsymbol{F}(\boldsymbol{q}_a) = -\big(\big\langle\!\!\big\langle \boldsymbol{P}, \boldsymbol{q}_a\big\rangle\!\!\big\rangle^\mu_Y\big)^{\rm T}. \tag{50c}$$

We then note that, for any $\boldsymbol{w}\in\boldsymbol{\mathcal{V}}$, the governing problem (18b) implies

$$\big\langle\!\!\big\langle \boldsymbol{w}, \boldsymbol{q}_a\big\rangle\!\!\big\rangle^\mu_Y = -\big\langle\!\!\big\langle \boldsymbol{w}, \boldsymbol{Q}_a\big\rangle\!\!\big\rangle^{\Delta\mu}_{B_a} + \Delta\boldsymbol{J}_a(\boldsymbol{w},\boldsymbol{P}_a) + \boldsymbol{J}(\boldsymbol{w},\boldsymbol{p}_a) + \Delta\boldsymbol{K}^Q_a(\boldsymbol{w}) - \Delta\boldsymbol{L}^Q_a(\boldsymbol{w}). \tag{50d}$$

Further, the following expansions hold for any $\boldsymbol{w}\in\boldsymbol{\mathcal{V}}$ that is smooth in a neighborhood of B_a:

$$\big\langle\!\!\big\langle \boldsymbol{w}, \boldsymbol{Q}_a\big\rangle\!\!\big\rangle^{\Delta\mu}_{B_a} = a^2(\boldsymbol{\nabla}\boldsymbol{w})^{\rm T}(\boldsymbol{z})\cdot\big\{\boldsymbol{A}\cdot\big(\boldsymbol{\nabla}\boldsymbol{Q}+\boldsymbol{I}\otimes\boldsymbol{P}\big) - \Delta\mu|\mathcal{B}|\boldsymbol{I}\otimes\boldsymbol{P}\big)\big\}(\boldsymbol{z}) + o(a^2), \tag{50e}$$

$$\begin{aligned} \Delta\boldsymbol{J}_a(\boldsymbol{w},\boldsymbol{P}_a) = a^2\Big\{ &\boldsymbol{w}^{\rm T}\otimes\boldsymbol{A}\cdot\big(\boldsymbol{\nabla}\boldsymbol{P}+\boldsymbol{I}\big) - \Delta\mu|\mathcal{B}|\big(\boldsymbol{w}^{\rm T}\otimes\boldsymbol{I} + (\boldsymbol{\nabla}\boldsymbol{w})^{\rm T}\otimes\boldsymbol{P}\big)\Big\}(\boldsymbol{z}) \\ &+ o(a^2), \end{aligned} \tag{50f}$$

$$\Delta\boldsymbol{K}^Q_a(\boldsymbol{w}) = a^2\Delta\mu|\mathcal{B}|\big\{\boldsymbol{w}^{\rm T}\otimes\boldsymbol{I}\big\}(\boldsymbol{z}) + o(a^2), \tag{50g}$$

$$\Delta\boldsymbol{L}^Q_a(\boldsymbol{w}) = a^2|Y|\Big\{\mathcal{D}\varrho^0\boldsymbol{w}\otimes\frac{\boldsymbol{\mu}^0}{\varrho^0} + \frac{\langle\rho\boldsymbol{w}\rangle}{\varrho^0}\otimes\Big(\mathcal{D}\boldsymbol{\mu}^0 - \mathcal{D}\varrho^0\frac{\boldsymbol{\mu}^0}{\varrho^0}\Big)\Big\}(\boldsymbol{z}) + o(a^2). \tag{50h}$$

Inserting these expressions into (50d) yields

$$\text{(50i)}\quad \langle\!\langle \boldsymbol{w}, \boldsymbol{q}_a \rangle\!\rangle_Y^{\mu} = a^2\Big\{ -(\boldsymbol{\nabla w})^{\mathrm{T}}\cdot\boldsymbol{A}\cdot\big(\boldsymbol{\nabla Q}+\boldsymbol{I}\otimes\boldsymbol{P}\big) + \boldsymbol{w}^{\mathrm{T}}\otimes\boldsymbol{A}\cdot\big(\boldsymbol{\nabla P}+\boldsymbol{I}\big)\Big\}(\boldsymbol{z}) + \boldsymbol{J}(\boldsymbol{w},\boldsymbol{p}_a)$$
$$- a^2|Y|\Big\{ \mathcal{D}\varrho^0\boldsymbol{w}\otimes\frac{\boldsymbol{\mu}^0}{\varrho^0} + \frac{\langle\rho\boldsymbol{w}\rangle}{\varrho^0}\otimes\Big(\mathcal{D}\boldsymbol{\mu}^0 - \mathcal{D}\varrho^0\frac{\boldsymbol{\mu}^0}{\varrho^0}\Big)\Big\}(\boldsymbol{z}) + o(a^2).$$

We now set $\boldsymbol{w}=\boldsymbol{P}$ in the above expression, so that (50c) yields

$$\text{(50j)}\quad \boldsymbol{F}(\boldsymbol{q}_a) = a^2\Big\{ \big(\boldsymbol{\nabla Q}+\boldsymbol{I}\otimes\boldsymbol{P}\big)^{\mathrm{T}}\cdot\boldsymbol{A}\cdot\boldsymbol{\nabla P} - \big(\boldsymbol{\nabla P}+\boldsymbol{I}\big)^{\mathrm{T}}\cdot\boldsymbol{A}\otimes\boldsymbol{P}\Big\}(\boldsymbol{z}) - \boldsymbol{J}^{\mathrm{T}}(\boldsymbol{P},\boldsymbol{p}_a)$$
$$+ a^2|Y|\Big\{ \mathcal{D}\varrho^0\boldsymbol{P}\otimes\frac{\boldsymbol{\mu}^0}{\varrho^0} + \frac{\langle\rho\boldsymbol{P}\rangle}{\varrho^0}\otimes\Big(\mathcal{D}\boldsymbol{\mu}^0 - \mathcal{D}\varrho^0\frac{\boldsymbol{\mu}^0}{\varrho^0}\Big)\Big\}^{\mathrm{T}}(\boldsymbol{z}) + o(a^2).$$

On substituting (50a), (50b), and (50j) into the formula (49) for modulus perturbation $\boldsymbol{\mu}_a^1-\boldsymbol{\mu}^1$, one finds

$$\boldsymbol{\mu}_a^1-\boldsymbol{\mu}^1 = a^2\Big\{ \mathcal{D}\varrho^0\boldsymbol{P}\otimes\frac{\boldsymbol{\mu}^0}{\varrho^0} + \frac{\boldsymbol{\varrho}^1}{\varrho^0}\otimes\Big(\mathcal{D}\boldsymbol{\mu}^0 - \mathcal{D}\varrho^0\frac{\boldsymbol{\mu}^0}{\varrho^0}\Big)$$
$$- |Y|^{-1}\big(\boldsymbol{\nabla P}+\boldsymbol{I}\big)^{\mathrm{T}}\cdot\boldsymbol{A}\cdot\boldsymbol{\nabla}\beta\otimes\frac{\boldsymbol{\mu}^0}{\varrho^0}\Big\}_{\mathrm{sym}}(\boldsymbol{z}),$$

thanks to the reciprocity identity (14). The claimed formula for $\mathcal{D}\boldsymbol{\mu}^1$ is finally established by using the expression for $\mathcal{D}\boldsymbol{\varrho}^1$ in the above expansion.

Density, second order. Here, we follow the approach used to derive $\mathcal{D}\boldsymbol{\varrho}_a^1$. On recalling the definition (8a) of $\boldsymbol{\varrho}^2$, we write

$$\text{(51)}\qquad \boldsymbol{\varrho}_a^2-\boldsymbol{\varrho}^2 \;=\; \langle\rho_a\boldsymbol{Q}_a-\rho\boldsymbol{Q}\rangle_{\mathrm{sym}} \;=\; \Delta\rho\langle\chi_{B_a}\boldsymbol{Q}_a\rangle_{\mathrm{sym}} + \langle\rho\boldsymbol{q}_a\rangle_{\mathrm{sym}}.$$

Then, the cell solution asymptotics (17b) and the formula for $\mathcal{D}\varrho^0(\boldsymbol{z})$ yield

$$\text{(52a)}\qquad \Delta\rho\langle\chi_{B_a}\boldsymbol{Q}_a\rangle \;=\; a^2|Y|^{-1}|\mathcal{B}|\Delta\rho\,\boldsymbol{Q}(\boldsymbol{z})+o(a^2) \;=\; \upsilon(a)\big\{\mathcal{D}\varrho^0\boldsymbol{Q}\big\}(\boldsymbol{z})+o(a^2),$$

while the leading contribution of $\langle\rho\boldsymbol{q}_a\rangle$ is evaluated by resorting to the adjoint problem (37a) with $w=\boldsymbol{q}_a$:

$$\text{(52b)}\qquad \langle\rho\boldsymbol{q}_a\rangle \;=\; \big\langle(\rho-\varrho^0)\boldsymbol{q}_a\big\rangle \;=\; |Y|^{-1}\langle\!\langle \boldsymbol{q}_a,\beta\rangle\!\rangle_Y^{\mu} \;=\; |Y|^{-1}\big(\langle\!\langle \beta,\boldsymbol{q}_a\rangle\!\rangle_Y^{\mu}\big)^{\mathrm{T}}.$$

The expansion of the above result is then given by (50i) with $\boldsymbol{w}=\beta$, i.e.,

$$\text{(52c)}\quad \langle\!\langle \beta, \boldsymbol{q}_a \rangle\!\rangle_Y^{\mu} = a^2\Big\{ -\boldsymbol{\nabla}\beta\cdot\boldsymbol{A}\cdot\big(\boldsymbol{\nabla Q}+\boldsymbol{I}\otimes\boldsymbol{P}\big) + \beta\boldsymbol{A}\cdot\big(\boldsymbol{\nabla P}+\boldsymbol{I}\big)\Big\}(\boldsymbol{z}) + \boldsymbol{J}(\beta,\boldsymbol{p}_a)$$
$$- a^2|Y|\Big\{ \mathcal{D}\varrho^0\beta\frac{\boldsymbol{\mu}^0}{\varrho^0} + \frac{\langle\rho\beta\rangle}{\varrho^0}\Big(\mathcal{D}\boldsymbol{\mu}^0 - \mathcal{D}\varrho^0\frac{\boldsymbol{\mu}^0}{\varrho^0}\Big)\Big\}(\boldsymbol{z}) + o(a^2),$$

where $\boldsymbol{J}(\beta,\boldsymbol{p}_a)$ can be expanded as

$$\text{(52d)}\quad \boldsymbol{J}(\beta,\boldsymbol{p}_a) = \langle\!\langle \boldsymbol{p}_a, \boldsymbol{X}[\beta]\rangle\!\rangle_Y^{\mu} = -\Big(\langle\!\langle \boldsymbol{X}[\beta],\boldsymbol{P}_a\rangle\!\rangle_{B_a}^{\Delta\mu} + \Delta\boldsymbol{F}_a(\boldsymbol{X}[\beta])\Big)^{\mathrm{T}}$$
$$= -a^2\Big\{\big(\boldsymbol{\nabla P}+\boldsymbol{I}\big)^{\mathrm{T}}\cdot\boldsymbol{A}\cdot\boldsymbol{\nabla X}[\beta]\Big\}(\boldsymbol{z})+o(a^2)$$

having used the adjoint problem (37b), the weak problem (18a) for $\boldsymbol{p}_a$, and expansion (35). The sought expression for $\mathcal{D}\boldsymbol{\varrho}^2$ is finally found by using (52a)–(52d) in (51).

Shear modulus, second order. The approach previously used for deriving $\mathcal{D}\boldsymbol{\mu}^1$ is used again. Recalling definition (15c) of $\boldsymbol{\mu}^2$, we thus need to evaluate the leading contribution as $a \to 0$ of

$$\boldsymbol{\mu}_a^2 - \boldsymbol{\mu}^2 = |Y|^{-1}\Big\{\Delta\boldsymbol{F}_a(\boldsymbol{R}_a) + \Delta\boldsymbol{K}_a^Q(\boldsymbol{Q}_a) + \boldsymbol{F}(\boldsymbol{r}_a) + \boldsymbol{K}^Q(\boldsymbol{q}_a)\Big\}_{\mathrm{sym}}. \tag{53}$$

First, similarly to (50a), we have

$$\begin{aligned}\Delta\boldsymbol{F}_a(\boldsymbol{R}_a) + \Delta\boldsymbol{K}_a^Q(\boldsymbol{Q}_a) &= \int_{B_a} \Delta\mu\big(\boldsymbol{\nabla}\boldsymbol{R}_a + \boldsymbol{I}\otimes\boldsymbol{Q}_a\big)^{\mathrm{T}}\,\mathrm{d}V \\ &= a^2\big(\boldsymbol{\nabla}\boldsymbol{R} + \boldsymbol{I}\otimes\boldsymbol{Q}\big)^{\mathrm{T}}(\boldsymbol{z})\cdot\boldsymbol{A} + o(a^2).\end{aligned} \tag{54a}$$

What remains to be determined is the leading contribution of $\boldsymbol{F}(\boldsymbol{r}_a) + \boldsymbol{K}^Q(\boldsymbol{q}_a)$. Following now-familiar lines, we have

$$\begin{aligned}&\big(\boldsymbol{F}(\boldsymbol{r}_a) + \boldsymbol{K}^Q(\boldsymbol{q}_a)\big)^{\mathrm{T}} \\ &\quad= -\big\langle\!\big\langle \boldsymbol{P}, \boldsymbol{r}_a\big\rangle\!\big\rangle_Y^{\mu} + \boldsymbol{K}^Q(\boldsymbol{q}_a)^{\mathrm{T}} \\ &\quad= \big\langle\!\big\langle \boldsymbol{P}, \boldsymbol{R}_a\big\rangle\!\big\rangle_{B_a}^{\Delta\mu} - \Delta\boldsymbol{J}_a(\boldsymbol{P},\boldsymbol{Q}_a) - \boldsymbol{J}(\boldsymbol{P},\boldsymbol{q}_a) - \Delta\boldsymbol{K}_a^R(\boldsymbol{P}) + \Delta\boldsymbol{L}_a^R(\boldsymbol{P}) + \boldsymbol{K}^Q(\boldsymbol{q}_a)^{\mathrm{T}}\end{aligned} \tag{54b}$$

by virtue of (18c) with $\boldsymbol{w} = \boldsymbol{P}$, and

$$\begin{aligned}&\big\langle\!\big\langle \boldsymbol{P}, \boldsymbol{R}_a\big\rangle\!\big\rangle_{B_a}^{\Delta\mu} \\ &\quad= a^2\Big\{(\boldsymbol{\nabla}\boldsymbol{P})^{\mathrm{T}}\cdot\boldsymbol{A}\cdot\big(\boldsymbol{\nabla}\boldsymbol{R} + \boldsymbol{I}\otimes\boldsymbol{Q}\big) - \Delta\mu|\mathcal{B}|(\boldsymbol{\nabla}\boldsymbol{P})^{\mathrm{T}}\otimes\boldsymbol{Q}\Big\}(\boldsymbol{z}) + o(a^2), \\ &\Delta\boldsymbol{J}_a(\boldsymbol{P},\boldsymbol{Q}_a) \\ &\quad= a^2\Big\{\boldsymbol{P}\otimes\boldsymbol{A}\cdot\big(\boldsymbol{\nabla}\boldsymbol{Q} + \boldsymbol{I}\otimes\boldsymbol{P}\big) - \Delta\mu|\mathcal{B}|\big(\boldsymbol{P}\otimes\boldsymbol{I}\otimes\boldsymbol{P} + (\boldsymbol{\nabla}\boldsymbol{P})^{\mathrm{T}}\otimes\boldsymbol{Q}\big)\Big\}(\boldsymbol{z}) + o(a^2),\end{aligned}$$

similar to expansions (50e) and (50f). Moreover, one finds that

$$\begin{aligned}-\boldsymbol{J}(\boldsymbol{P},\boldsymbol{q}_a) + \boldsymbol{K}^Q(\boldsymbol{q}_a)^{\mathrm{T}} &= -\boldsymbol{J}(\boldsymbol{P},\boldsymbol{q}_a) + \big(\big\langle\!\big\langle \boldsymbol{q}_a, \boldsymbol{Q}\big\rangle\!\big\rangle_Y^{\mu}\big)^{\mathrm{T}} + \boldsymbol{L}^Q(\boldsymbol{q}_a)^{\mathrm{T}} - \boldsymbol{J}(\boldsymbol{q}_a,\boldsymbol{P})^{\mathrm{T}} \\ &= \big\langle\!\big\langle \boldsymbol{Q}, \boldsymbol{q}_a\big\rangle\!\big\rangle_Y^{\mu} + \frac{\boldsymbol{\mu}^0}{\varrho^0}\otimes\big\langle\!\big\langle \beta, \boldsymbol{q}_a\big\rangle\!\big\rangle_Y^{\mu},\end{aligned}$$

thanks to the weak problem (11b) for $\boldsymbol{Q}$, property (14) of $\boldsymbol{J}$, and the adjoint problem (37a) for β. On recalling (52c) and retracing the derivation of $\mathcal{D}\boldsymbol{\varrho}^2$, we have

$$\big\langle\!\big\langle \beta, \boldsymbol{q}_a\big\rangle\!\big\rangle_Y^{\mu} = a^2|Y|\big(\mathcal{D}\boldsymbol{\varrho}^2 - \mathcal{D}\varrho^0\boldsymbol{Q}\big)(\boldsymbol{z}) + o(a^2),$$

while $\big\langle\!\big\langle \boldsymbol{Q}, \boldsymbol{q}_a\big\rangle\!\big\rangle_Y^{\mu}$ can be evaluated via (50i) with $\boldsymbol{w} = \boldsymbol{Q}$. As a result,

$$\begin{aligned}&-\boldsymbol{J}(\boldsymbol{P},\boldsymbol{q}_a) + \boldsymbol{K}^Q(\boldsymbol{q}_a)^{\mathrm{T}} \\ &= a^2\Big\{-\boldsymbol{\nabla}\boldsymbol{Q}^{\mathrm{T}}\cdot\boldsymbol{A}\cdot\big(\boldsymbol{\nabla}\boldsymbol{Q} + \boldsymbol{I}\otimes\boldsymbol{P}\big) + \boldsymbol{Q}^{\mathrm{T}}\otimes\boldsymbol{A}\cdot\big(\boldsymbol{\nabla}\boldsymbol{P} + \boldsymbol{I}\big)\Big\}(\boldsymbol{z}) + \boldsymbol{J}(\boldsymbol{Q},\boldsymbol{p}_a) \\ &\qquad + a^2|Y|\Big\{\frac{\boldsymbol{\mu}^0}{\varrho^0}\otimes\big(\mathcal{D}\boldsymbol{\varrho}^2 - \mathcal{D}\varrho^0\boldsymbol{Q}\big) - \mathcal{D}\varrho^0\boldsymbol{Q}\otimes\frac{\boldsymbol{\mu}^0}{\varrho^0} - \frac{\boldsymbol{\varrho}^2}{\varrho^0}\otimes\Big(\mathcal{D}\boldsymbol{\mu}^0 - \mathcal{D}\varrho^0\frac{\boldsymbol{\mu}^0}{\varrho^0}\Big)\Big\}(\boldsymbol{z}).\end{aligned}$$

Next, from definitions (13) applied to both the unperturbed and perturbed cells, we have

$$
\begin{aligned}
&-\Delta\boldsymbol{K}_a^R(\boldsymbol{P})+\Delta\boldsymbol{L}_a^R(\boldsymbol{P})\\
&=a^2\Big\{|\mathcal{B}|\boldsymbol{P}\otimes\Big(\Delta\rho\frac{\boldsymbol{\mu}^0}{\varrho^0}-\Delta\mu\boldsymbol{I}\Big)\otimes\boldsymbol{P}+\frac{|Y|}{\varrho^0}\Big\langle\rho\boldsymbol{P}\otimes\Big(\mathcal{D}\boldsymbol{\mu}^0-\mathcal{D}\varrho^0\frac{\boldsymbol{\mu}^0}{\varrho^0}\Big)(\boldsymbol{z})\otimes\boldsymbol{P}\Big\rangle\Big\}(\boldsymbol{z})\\
&\qquad+\boldsymbol{L}^R(\boldsymbol{p}_a)-\boldsymbol{K}^R(\boldsymbol{p}_a)+o(a^2).
\end{aligned}
$$

On deploying the weak problem (11c) with $w=\boldsymbol{p}_a$ and recalling (46b), one finds

$$
\begin{aligned}
\boldsymbol{L}^R(\boldsymbol{p}_a)-\boldsymbol{K}^R(\boldsymbol{p}_a)&=\boldsymbol{J}(\boldsymbol{p}_a,\boldsymbol{Q})-\big\langle\!\big\langle\boldsymbol{p}_a,\boldsymbol{R}\big\rangle\!\big\rangle_Y^{\mu}\\
&=\boldsymbol{J}(\boldsymbol{p}_a,\boldsymbol{Q})+a^2\big\{\big(\boldsymbol{\nabla P}+\boldsymbol{I}\big)^{\mathrm{T}}\cdot\boldsymbol{A}\cdot\boldsymbol{\nabla R}\big\}(\boldsymbol{z})+o(a^2).
\end{aligned}
$$

Collecting the above expansions of the terms on the right-hand side of (54b) and performing symmetrization (7), we find

(54c)

$$
\begin{aligned}
&\big[\boldsymbol{F}(\boldsymbol{r}_a)+\boldsymbol{K}^Q(\boldsymbol{q}_a)\big]_{\mathrm{sym}}\\
&=a^2\Big[\Big\{\big(2\boldsymbol{\nabla P}+\boldsymbol{I}\big)^{\mathrm{T}}\cdot\boldsymbol{A}\cdot\big(\boldsymbol{\nabla R}+\boldsymbol{I}\otimes\boldsymbol{Q}\big)-\big(\boldsymbol{\nabla Q}+\boldsymbol{I}\otimes\boldsymbol{P}\big)^{\mathrm{T}}\cdot\boldsymbol{A}\cdot\big(\boldsymbol{\nabla Q}+\boldsymbol{I}\otimes\boldsymbol{P}\big)\Big\}(\boldsymbol{z})\\
&\qquad+|Y|\frac{\boldsymbol{\mu}^0}{\varrho^0}\otimes\Big\{\mathcal{D}\boldsymbol{\varrho}^2+\mathcal{D}\varrho^0\big(\boldsymbol{P}\otimes\boldsymbol{P}-2\boldsymbol{Q}\big)\Big\}(\boldsymbol{z})\\
&\qquad+|Y|\frac{1}{\varrho^0}\Big\{\big(\big\langle\rho\boldsymbol{P}\otimes\boldsymbol{P}\big\rangle-\boldsymbol{\varrho}^2\big)\otimes\Big(\mathcal{D}\boldsymbol{\mu}^0-\mathcal{D}\varrho^0\frac{\boldsymbol{\mu}^0}{\varrho^0}\Big)\Big\}(\boldsymbol{z})\Big]_{\mathrm{sym}}+\,o(a^2).
\end{aligned}
$$

The sought for formula for $\mathcal{D}\boldsymbol{\mu}^2$ as in Theorem 5 then follows by substituting (54a) and (54c) into (53).

7. Numerical illustrations. In what follows, we provide two examples exercising the sensitivity formulas in Theorem 5 for simple unit cells and perturbation shapes. The computations of the cell and adjoint functions is performed using the finite element platform FreeFem++ [16, 19].

7.1. Fast computation of the sensitivity coefficients. By neglecting the $o(v(a))$ remainder in (20), one obtains the leading-order perturbation of the coefficients of homogenization ($\varrho^0,\boldsymbol{\mu}^0$, etc.) due to insertion of a small inhomogeneity inside the reference unit cell. Note that such an approximation is also relevant to small-volume-fraction composites [12, 2], in which context the expansion has been extended to higher orders [18] in order to handle $O(1)$ volume fractions. To our knowledge, however, such computations are normally performed for biphased materials (i.e., for inclusions in a homogeneous matrix) and not for additional inclusions nucleating in an *already periodic* medium (see also Remark 6).

As an illustration, we show in Figure 1 the error made by the approximation $\boldsymbol{\mu}^0+\frac{a^2}{|Y|}\mathcal{D}\boldsymbol{\mu}^0(\boldsymbol{z})$ of $\boldsymbol{\mu}_a^0$ for a reference "chessboard" unit cell perturbed by a "stiff" ellipsoidal inclusion with semiaxes $(a,0.2a)$, centered at $\boldsymbol{z}=(0.25,0.25)$. It is seen that even for values of a close to 0.25 (this value being the limit for which the smoothness assumptions inside B_a cease to hold), the maximum approximation error remains below 1%. Note also that this error is $O(a^4)$, instead of expected $O(a^3)$; on the basis

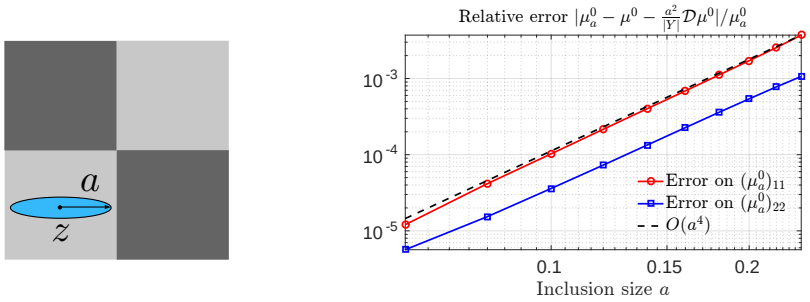

FIG. 1. *Approximation of $\boldsymbol{\mu}_a^0$ by its leading-order topological expansion for a chessboard unit cell perturbed by an ellipsoidal inclusion with $\Delta\mu = 1$ and semiaxes $(a, 0.2a)$, centered at $\boldsymbol{z} = (0.25, 0.25)$. Left: perturbed unit cell where the light (resp., dark) gray indicates $\mu = 1$ (resp., $\mu = 2$). Right: relative error made by the leading-order approximation of a $\boldsymbol{\mu}_a^0$ in terms of its diagonal entries. The mass density of all constituents inside the perturbed unit cell is $\rho = 1$.*

of a recent higher-order TS analysis [7], we believe (without proof for now) that this holds for any *centrally symmetric* inclusion.

Here it is useful to recall that evaluating $\boldsymbol{\mu}^0 + \frac{a^2}{|Y|}\mathcal{D}\boldsymbol{\mu}^0$ requires (i) computing $\boldsymbol{P}$ and $\boldsymbol{\mu}^0$ for the reference cell *once and for all*; (ii) computing the polarization tensor $\boldsymbol{A}(\mu(\boldsymbol{z}), \Delta\mu, \mathcal{B})$ for a given material contrast $\Delta\mu$, shape $\mathcal{B}$, and each location $\boldsymbol{z}$ of the inclusion; and (iii) scaling the result $\mathcal{D}\boldsymbol{\mu}^0(\boldsymbol{z}) = \{(\boldsymbol{\nabla P} + \boldsymbol{I})^{\mathrm{T}} \cdot \boldsymbol{A} \cdot (\boldsymbol{\nabla P} + \boldsymbol{I})\}(\boldsymbol{z})$ by $\frac{a^2}{|Y|}$ for given a (provided that the smoothness assumptions on μ inside B_a hold). This computational effort should be compared to that underpinning the exact evaluation of $\boldsymbol{\mu}_a^0$, which requires solving a new cell function, $\boldsymbol{P}_a$, for each choice of inclusion, i.e., each set $(\boldsymbol{z}, \mathcal{B}, \Delta\mu, a)$, that could be very costly for complex (reference and perturbed) cell configurations.

Remark 8. Step (ii) above requires a minimal computational effort when the analytical expression for $\boldsymbol{A}$ is known—as is the case with ellipsoidal inclusions; see Remark 5. In situations when $\mathcal{B}$ is arbitrary, on the other hand, step (ii) necessitates solving the free-space transmission problem (30) anew for each value taken by the ratio $\Delta\mu/\mu(\boldsymbol{z})$. For piecewise-homogeneous reference cells, this entails only a few evaluations; considering the chessboard unit cell in Figure 1 for example, the evaluation of $\boldsymbol{A}$ for arbitrary $\mathcal{B}$ and any $\boldsymbol{z}$ would (given $\Delta\mu$) require only two solutions of (30).

7.2. Subwavelength sensing of periodic structures. We set up the second example as a *defect identification* procedure, where a "defective" chessboard-like material (hereon referred to as the *manufactured* material) is interrogated by plane waves. The sensory data, used to probe for defects, are the phase velocities of such waves for several directions of incidence—as captured over a low-frequency (and thus long-wavelength) range. In the identification procedure, the experimental phase velocities are compared to their reference values, computed for the *designed* material. The observed anisotropic dispersion, which is a key feature of the sensory data, is captured only via *second-order* homogenization, so that both zero-order ($\mathcal{D}\varrho^0$, $\mathcal{D}\boldsymbol{\mu}^0$) and second-order ($\mathcal{D}\boldsymbol{\varrho}^2$, $\mathcal{D}\boldsymbol{\mu}^2$) coefficient sensitivities given by Theorem 5 are needed to interpret the data. This is shown next.

Topological sensitivity of the phase velocity. We first recall the second-order, mean field equation

$$\boldsymbol{\mu}^0 : \boldsymbol{\nabla}^2 U + \varepsilon^2 \boldsymbol{\mu}^2 : \boldsymbol{\nabla}^4 U + \omega^2 \big(\varrho^0 U + \varepsilon^2 \boldsymbol{\varrho}^1 : \boldsymbol{\nabla}^2 U \big) \;=\; o(\varepsilon^3), \tag{55}$$

according to (16). To characterize the dispersion of a homogenized material, we set the mean field as a plane wave propagating in direction $\boldsymbol{d} = (\cos\theta, \sin\theta)$ with wavenumber k, i.e., $U(\boldsymbol{x}) \propto e^{\mathrm{i}k\boldsymbol{d}\cdot\boldsymbol{x}}$. On substituting this plane wave into (55) and neglecting the $o(\varepsilon^3)$ remainder, one obtains the characteristic relation

$$\varepsilon^2(\boldsymbol{\mu}^2 : \boldsymbol{d}^{\otimes 4})k^4 - \left((\boldsymbol{\mu}^0 + \varepsilon^2\omega^2\boldsymbol{\varrho}^1) : \boldsymbol{d}^{\otimes 2}\right)k^2 + \omega^2\varrho^0 \;=\; 0 \tag{56}$$

(with $\boldsymbol{d}^{\otimes 2} := \boldsymbol{d}\otimes\boldsymbol{d}$ and $\boldsymbol{d}^{\otimes 4} := \boldsymbol{d}\otimes\boldsymbol{d}\otimes\boldsymbol{d}\otimes\boldsymbol{d}$) which in turn yields the anisotropic dispersion formula

$$c(k,\boldsymbol{d}) \;=\; \frac{\omega(k,\boldsymbol{d})}{k} \;=\; \left(\frac{\boldsymbol{\mu}^0 : \boldsymbol{d}^{\otimes 2} - \varepsilon^2 k^2 \boldsymbol{\mu}^2 : \boldsymbol{d}^{\otimes 4}}{\varrho^0 - \varepsilon^2 k^2 \boldsymbol{\varrho}^1 : \boldsymbol{d}^{\otimes 2}}\right)^{1/2}. \tag{57}$$

For perturbed unit cells, the expansion $c_a = c + v(a)\mathcal{D}c + o(v(a))$ (i.e., (20) for $f_a = c_a$) holds, and $\mathcal{D}c$ is expressed in terms of the sensitivities of the homogenized coefficients:

$$\begin{aligned}\mathcal{D}c(k,\boldsymbol{d},\boldsymbol{z}) \\ = \frac{\left[\mathcal{D}\boldsymbol{\mu}^0 : \boldsymbol{d}^{\otimes 2} - \varepsilon^2 k^2 \mathcal{D}\boldsymbol{\mu}^2 : \boldsymbol{d}^{\otimes 4} - (c(k,\boldsymbol{d}))^2\left(\mathcal{D}\varrho^0 - \varepsilon^2 k^2 \mathcal{D}\boldsymbol{\varrho}^1 : \boldsymbol{d}^{\otimes 2}\right)\right](\boldsymbol{z})}{2\left(\varrho^0 - \varepsilon^2 k^2 \boldsymbol{\varrho}^1 : \boldsymbol{d}^{\otimes 2}\right)}.\end{aligned} \tag{58}$$

Quasi-static and dynamic misfit functionals. In what follows, the manufactured material is illuminated by plane waves with wavenumbers $(k_p)_{p=1..N_k}$ propagating in directions $(\theta_j)_{j=1..N_\theta}$. The sensory data are thus the phase velocities $c^{\mathrm{obs}}(k_p, \boldsymbol{d}_j)$, where $\boldsymbol{d}_j = (\cos\theta_j, \sin\theta_j)$. For given wavenumber and direction of incidence $(k,\boldsymbol{d})$, we define the cost functional

$$J(k,\boldsymbol{d}) \;=\; \frac{1}{2}\left[c(k,\boldsymbol{d}) - c^{\mathrm{obs}}(k,\boldsymbol{d})\right]^2, \tag{59}$$

quantifying the misfit between the designed and observed phase velocities. We also define the dynamic cost functional J^{dyn}, extracting the effects of dispersion, as

$$J^{\mathrm{dyn}}(k,\boldsymbol{d}) = \frac{1}{2}\left[\Delta c(k,\boldsymbol{d}) - \Delta c^{\mathrm{obs}}(k,\boldsymbol{d})\right]^2, \quad \Delta c(k,\boldsymbol{d}) \;=\; c(k,\boldsymbol{d}) - c(k_{\min},\boldsymbol{d}), \tag{60}$$

where $k_{\min}$ is the smallest observed wavenumber (typically, $k_{\min} = k_1 > 0$). The TSs of these two misfit functionals depend on the sensitivity $\mathcal{D}c$ given by (58) as

$$\begin{aligned}\mathcal{D}J(k,\boldsymbol{d},\boldsymbol{z}) \;&=\; \left(c(k,\boldsymbol{d}) - c^{\mathrm{obs}}(k,\boldsymbol{d})\right)\mathcal{D}c(k,\boldsymbol{d},\boldsymbol{z}), \\ \mathcal{D}J^{\mathrm{dyn}}(k,\boldsymbol{d},\boldsymbol{z}) \;&=\; \left(\Delta c(k,\boldsymbol{d}) - \Delta c^{\mathrm{obs}}(k,\boldsymbol{d})\right)\left(\mathcal{D}c(k,\boldsymbol{d},\boldsymbol{z}) - \mathcal{D}c(k_{\min},\boldsymbol{d},\boldsymbol{z})\right).\end{aligned} \tag{61}$$

In this setting, we finally define the aggregate *quasi-static* and *dynamic* cost functionals as

$$\mathcal{J}^{\mathrm{stat}} \;=\; \sum_{j=1}^{N_\theta} J(k_{\min},\boldsymbol{d}_j) \qquad \text{and} \qquad \mathcal{J}^{\mathrm{dyn}} \;=\; \sum_{j=1}^{N_\theta}\sum_{p=1}^{N_k} J^{\mathrm{dyn}}(k_p,\boldsymbol{d}_j), \tag{62}$$

whose sensitivities $\mathcal{D}\mathcal{J}^{\mathrm{stat}}$ and $\mathcal{D}\mathcal{J}^{\mathrm{dyn}}$ are computed by way of (61).

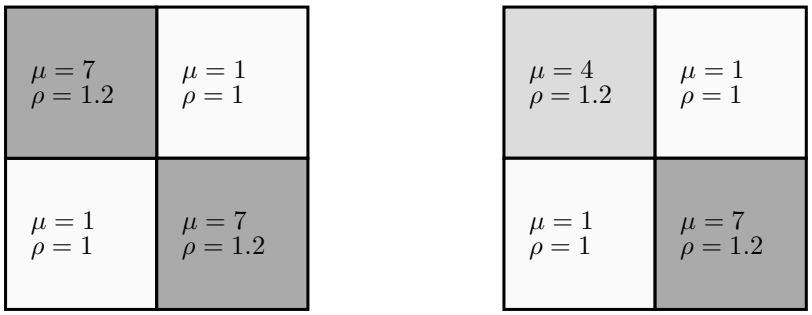

FIG. 2. *Designed (left) and manufactured (right)* 1×1 *unit cell of a chessboard-like material.*

Example: Incorrectly manufactured chessboard-like material. The chessboard-like material, *as designed*, is depicted in the left panel of Figure 2, featuring the coefficient ratios $\mu_{\max} = 7\mu_{\min}$ and $\rho_{\max} = 1.2\rho_{\min}$. For this configuration, the coefficients of homogenization are computed as

$$\begin{aligned} &\varrho^0 = 1.1\rho_{\min}, && \boldsymbol{\mu}^0 = 2.65\mu_{\min}\boldsymbol{I}, \\ &\boldsymbol{\varrho}^1 = 1.15 \times 10^{-4}\rho_{\min}\boldsymbol{I}, && \boldsymbol{\mu}^2 : \begin{cases} \mu^2_{1111} = \mu^2_{2222} = 4.36 \times 10^{-3}\mu_{\min}, \\ \mu^2_{1122} = 1.20 \times 10^{-2}\mu_{\min}, \\ \mu^2_{1112} = \mu^2_{1222} = 0. \end{cases} \end{aligned} \tag{63}$$

The chessboard-like material, *as manufactured*, has a defective top-left box in each unit cell, where $\mu = 4$ instead of $\mu = 7$ as shown in the right panel of Figure 2.

To identify and localize the defect, the plane-wave probing grid has $N_\theta = 7$ incident directions $\theta_j = (j-3)\pi/8$, $j = \overline{1, N_\theta}$, and $N_k = 10$ wavenumbers $k_p = 2p\,\pi/30$, $p = \overline{1, N_k}$. With such hypotheses, the *shortest wavelength* used to probe the periodic structure is roughly $\lambda_{\min} = 2\pi/k_{N_k} \simeq \pi$ which, relative to the 1×1 size of the unit cell, implies sensing *below* the classical diffraction limit. With reference to the above sensing grid, the left panel in Figure 3 compares the second-order approximation of the phase velocity (57) with the *numerical* values of $c(k, \boldsymbol{d})$—as computed via the Floquet–Bloch transform [27]—for both the designed and manufactured unit cell configuration. As can be seen from the display, the second-order approximation of anisotropic dispersion for the designed material agrees reasonably well with numerical simulations, noting that the small discrepancy between the two is attributed primarily to a limited accuracy of the numerical (Floquet–Bloch) solution due to a combination of material discontinuities inside the unit cell (which slow down the numerical convergence) and computer memory limitations. In contrast, there is a notable discrepancy between the dispersive characteristics of the designed and manufactured material, which justifies the use of $\mathcal{J}^{\text{stat}}$ as a basis for (periodic) defect identification. From the results for $\Delta c(k, \boldsymbol{d})$ shown in the right panel of Figure 3, this is also the case with $\mathcal{J}^{\text{dyn}}$, noting that some of the probing directions are in this case redundant owing to inherent symmetries of the designed and manufactured unit cell.

In this setting, the quasistatic sensitivity $\mathcal{DJ}^{\text{stat}}(\boldsymbol{z})$ serves as an indicator of the relative stiffness of the manufactured material (stiffer or softer than the designed material), via the sign of $\Delta\mu$ which gives $\mathcal{DJ}^{\text{stat}} < 0$. In this vein, Figure 4 plots $\mathcal{DJ}^{\text{stat}}(\boldsymbol{z})$ over the support of the unit cell, assuming both $\Delta\mu = 1$ (left panel) and $\Delta\mu = -1$ (right panel). To simplify the discussion, the analysis assumes prior

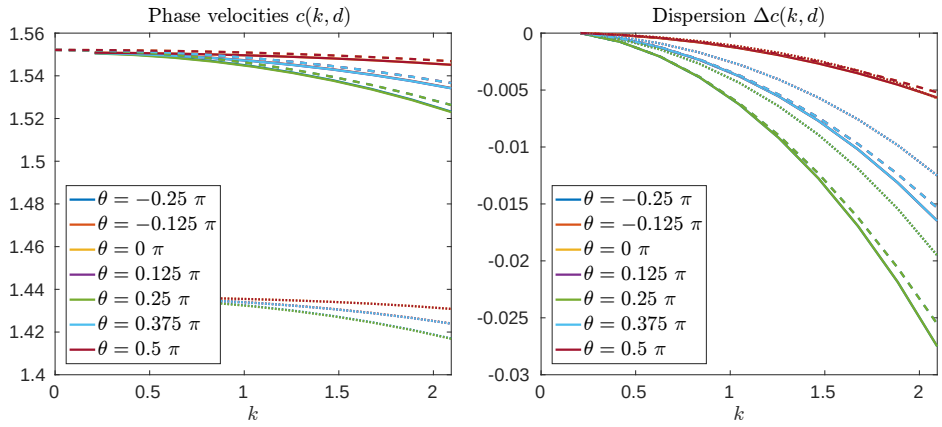

FIG. 3. *Left: phase velocity* $c(k,\boldsymbol{d})$ *for the* designed *chessboard material (homogenized model—dashed, numerical values—solid), and* manufactured *chessboard material (numerical values—dotted). Right: anisotropic dispersion shown in terms of* $\Delta c(k,\boldsymbol{d}) = c(k,\boldsymbol{d}) - c(k_{\min},\boldsymbol{d})$. *Note that the results for directions* $\theta = \{0,\pi/2\}$ *coincide, as do those for directions* $\theta = \{-\pi/4,\pi/4\}$ *and* $\theta = \{-\pi/8,\pi/8,3\pi/8\}$.

knowledge of the fact that the mass density of the unit cell is manufactured exactly (see Figure 1) by letting $\Delta\rho = 0$. For $\Delta\mu = 1$, we see that $\mathcal{DJ}^{\text{stat}} \geqslant 0$ everywhere; in other words, adding a stiff inclusion to the designed unit cell anywhere would only increase the quasistatic misfit functional. On the contrary, for $\Delta\mu = -1$ one has $\mathcal{DJ}^{\text{stat}} \leqslant 0$ everywhere (as expected) since the manufactured material is *softer* than designed. In light of its sign semidefiniteness for given $\Delta\mu$, however, $\mathcal{DJ}^{\text{stat}}$ appears to have *no localizing capabilities* in that it cannot locate (even approximately) the support of a periodic defect inside the unit cell.

To tackle the latter drawback, we deploy the dynamic sensitivity $\mathcal{DJ}^{\text{dyn}}$ as a sensing lens in Figure 5, taking $\Delta\mu = -1$ thanks to the quasi-static result. Indeed, the dynamic sensitivity appears to serve as a *remarkable defect locator*: $\mathcal{DJ}^{\text{dyn}} \geqslant 0$ over most of the intact quarter-cells—which are manufactured correctly (except near material interfaces, where the sensitivities tend to localize), while $\mathcal{DJ}^{\text{dyn}} \leqslant 0$ over the entire defective upper-left quarter-cell as expected, but also over the lower-right quarter-cell. The latter, however, should not be surprising, since (for the manufactured material at hand) the support of the unit cell could be chosen such that the defective quatrer-cell appears as either upper-left or lower-right. In light of this result, the long-wavelength sensing of periodic defects or perturbations could be established by (i) considering the *anisotropic dispersion*-based cost functionals (62), (ii) choosing the sign of $\Delta\mu$ so that $\mathcal{DJ}^{\text{stat}}(\boldsymbol{z}) \leqslant 0$ everywhere, and (iii) identifying the support of a perturbation inside the unit cell via regions where $\mathcal{DJ}^{\text{dyn}}(\boldsymbol{z}) \leqslant 0$.

8. Summary. In this work, explicit formulas are derived for the sensitivities of the second-order macroscopic model for waves in periodic media due to topological perturbations of the microscopic unit cell. The sensitivity analysis focuses on the tensorial (mass density and elastic modulus) coefficients in the governing field equation, featuring the macroscopic dispersive effects brought about by the presence of the macrostructure. The results demonstrate that the sought derivatives are expressible in terms of (i) three unit cell solutions featured by the (unperturbed) macroscopic model; (ii) two adoint-field solutions stemming from the mass density variations in the

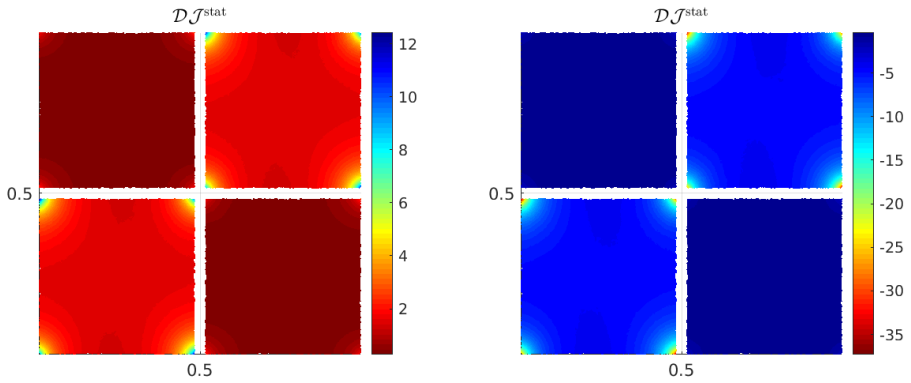

FIG. 4. *Distribution of quasi-static sensitivity* $\mathcal{DJ}^{\mathrm{stat}}(\boldsymbol{z})$ *over the unit cell assuming* $\Delta\mu = 1$ *(left) and* $\Delta\mu = -1$ *(right). The near-interface points are omitted from the plot.*

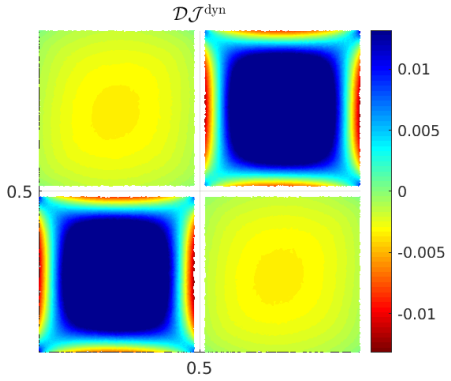

FIG. 5. *Distribution of dynamic sensitivity* $\mathcal{DJ}^{\mathrm{dyn}}(\boldsymbol{z})$ *over the unit cell assuming* $\Delta\mu = -1$. *The near-interface points are omitted from the plot, and a threshold is applied to the most positive TS values (as only their sign is of interest) so that the color scale is symmetric around* 0.

unperturbed periodic medium; and (iii) the usual polarization tensor, appearing in the TS studies of nonperiodic media, that synthesizes the geometric and material characteristics of a point-like perturbation. The proposed developments may especially aid (a) the design of periodic solids, focused on manipulating the long-wavelength material response via microstructure-generated effects of dispersion and anisotropy, and (b) subwavelength sensing of periodic defects or perturbations. Finally, we expect the proposed idea to also work in more general situations involving, e.g., in-plane (elastodynamic) Navier equations, albeit at a cost of notably heavier algebra.

Appendix A. Proof of Lemma 2. The proof of the claim is very similar to that in [8, Prop. 2], so we highlight only the main steps.

On writing the linear combination (25)$-a\times$(28) of the relevant VIEs, the inner expansion error $\boldsymbol{\delta}_a := \boldsymbol{P}_a(\boldsymbol{x}) - \boldsymbol{P}(\boldsymbol{z}) - a\big\{\,[\boldsymbol{U}(\bar{\boldsymbol{x}})\cdot\big(\boldsymbol{\nabla P}+\boldsymbol{I}\big)(\boldsymbol{z}) - \bar{\boldsymbol{x}}\,\big\}]$ is found to satisfy the integral equation $\big(\mathcal{I}+\mathcal{L}_a\big)\boldsymbol{\delta}_a(\boldsymbol{x}) = \boldsymbol{\gamma}_a(\boldsymbol{x})$, where

$$\boldsymbol{\gamma}_a(\boldsymbol{x}) := \boldsymbol{P}(\boldsymbol{x}) - \boldsymbol{P}(\boldsymbol{z}) - a\bar{\boldsymbol{x}}\cdot\boldsymbol{\nabla P}(\boldsymbol{z}) \\ -\Delta\mu\Big\{\int_{B_a}\boldsymbol{\nabla}_1 G_{\mathrm{c}}(\boldsymbol{y},\boldsymbol{x})\cdot\boldsymbol{\nabla U}\Big(\frac{\boldsymbol{y}-\boldsymbol{z}}{a}\Big)\,\mathrm{d}V(\boldsymbol{y})\Big\}\cdot(\boldsymbol{\nabla P}+\boldsymbol{I})(\boldsymbol{z}). \tag{64}$$

The claimed estimate is then established by showing that, for a sufficiently small,

we have (i) the bounded invertibility of $\mathcal{I}+\mathcal{L}_a:\ H^1(B_a)\to\ H^1(B_a)$, uniformly in a, and (ii) the estimate $\|\boldsymbol{\gamma}_a\|_{H^1(B_a)}\le Ca^2$. We first introduce the decomposition $\mathcal{L}_a=\mathcal{L}_a^\infty+\mathcal{L}_a^{\mathrm{c}}$ induced by decomposition (22) of the Green's kernel. In this setting, the proof of (i) follows from a Neumann series argument by showing first that $\mathcal{I}+\mathcal{L}_a^\infty$ is invertible with bounded inverse, the bound being uniform in a for sufficiently small a, and second that $\|\mathcal{L}_a^{\mathrm{c}}-\mathcal{L}_a^\infty\|=O(a)$. Concerning the proof of (ii), we have that $\|\boldsymbol{P}(\boldsymbol{x})-\boldsymbol{P}(\boldsymbol{z})-a\bar{\boldsymbol{x}}\cdot\boldsymbol{\nabla}\boldsymbol{P}(\boldsymbol{z})\|_{H^1(B_a)}=O(a^2)$ as the norm of the Taylor-expansion remainder of a function $\boldsymbol{x}\mapsto\boldsymbol{P}(\boldsymbol{x})$, which is smooth in a neighborhood of $\boldsymbol{x}=\boldsymbol{z}$. The remaining (integral) part of $\boldsymbol{\gamma}_a$ is also $O(a^2)$ by virtue of the kernel $G_{\mathrm{c}}(\boldsymbol{y},\boldsymbol{x})$ being smooth in a neighborhood of $(\boldsymbol{x},\boldsymbol{y})=(\boldsymbol{z},\boldsymbol{z})$.

Appendix B. Proof of Lemma 3. Equation (25), treated as a representation formula, gives $\boldsymbol{p}_a=-\mathcal{L}_a(\boldsymbol{P}_a+\boldsymbol{x})$ in $B_a\cup(Y\setminus\overline{B_a})$. With $\mathcal{L}_\infty$ given by (29), $\boldsymbol{\delta}_a$, $\mathcal{L}_a^\infty$, and $\mathcal{L}_a^{\mathrm{c}}$ as given in Appendix A, and $\boldsymbol{P}_1$ as introduced in (26), we have

$$\boldsymbol{p}_a=-a\mathcal{L}_\infty(\boldsymbol{P}_1+\bar{\boldsymbol{x}})-\mathcal{L}_a^\infty\boldsymbol{\delta}_a-\mathcal{L}_a^{\mathrm{c}}(\boldsymbol{P}_a+\boldsymbol{x})=:\boldsymbol{p}_a^1+\boldsymbol{p}_a^2+\boldsymbol{p}_a^3.$$

We readily have that $\|\boldsymbol{p}_a^2\|_{L^2(Y)}=O(a^2)$ (by virtue of Lemma 2 and the boundedness of $\mathcal{L}_a^\infty$, uniform in a, as a $H^1(B_a)\to L^2(Y)$ operator) and that $\|\boldsymbol{p}_a^3\|_{L^2(Y)}=O(a^2)$ (because the smoothness of the kernel $\boldsymbol{\nabla}_1G_{\mathrm{c}}$ in $Y\times Y$, together with $|B_a|=O(a^2)$, implies $\boldsymbol{p}_a^3=O(a^2)$ pointwise in Y). Regarding $\boldsymbol{p}_a^1$, on the other hand, one finds by the rescaling of coordinates that

$$\begin{aligned}&\|\boldsymbol{p}_a^1(\boldsymbol{x})\|_{L^2(Y)}^2\\&\quad=a^4\int_{(Y-\boldsymbol{z})/a}\Big|\Delta\mu\int_B\boldsymbol{\nabla}G_\infty\big(\bar{\boldsymbol{y}}-\bar{\boldsymbol{x}};\mu(\boldsymbol{z})\big)\cdot\boldsymbol{\nabla}(\boldsymbol{P}_1+\bar{\boldsymbol{y}})\,\mathrm{d}V(\bar{\boldsymbol{y}})\Big|^2\,\mathrm{d}V(\bar{\boldsymbol{x}}).\end{aligned}$$

Since $\boldsymbol{\nabla}G_\infty\big(\bar{\boldsymbol{y}}-\bar{\boldsymbol{x}};\mu(\boldsymbol{z})\big)=O(|\bar{\boldsymbol{x}}|^{-1})$ as $|\bar{\boldsymbol{x}}|\to\infty$, the above integral over $(Y-\boldsymbol{z})/a$ can be shown to be of order $O(\ln a)$ as $a\to0$. Consequently, $\|\boldsymbol{p}_a^1(\boldsymbol{x})\|_{L^2(Y)}=o(a)$, which completes the proof of the lemma.

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