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## ASYMPTOTIC ANALYSIS AND POLARIZATION MATRICES

#### S.A. NAZAROV, J. SOKOLOWSKI, AND M. SPECOVIUS-NEUGEBAUER

ABSTRACT. Polarization matrices are considered for the elasticity boundary value problems in two and three spatial dimensions. The matrices are introduced in the framework of asymptotic analysis for boundary value problems depending on small geometrical parameter, it is the size of an elastic inclusion or a defect (cavity, crack) in an elastic body. Our analysis is performed for some representative classes of boundary value problems, however the method is general and can be applied to the modelling and optimization in structural mechanics or for coupled models like piezoelectricity. The explicit properties obtained for polarization matrices are useful for mathematical analysis and for numerical solution of control, inverse and shape optimization problems with mathematical models derived by the asymptotic analysis in singularly perturbed geometrical domains. The analysis is performed by some different techniques including asymptotics in unbounded domains, singular perturbations and shape sensitivity. In particular, since the polarization matrices can be identified for some classes of shapes, we provide the formulae for numerical evaluation of such matrices for *nearby shapes* by means of the shape sensitivity analysis.

#### 1. INTRODUCTION

The asymptotic analysis in singularly perturbed geometrical domains is a tool of mathematical modeling in elasticity or for coupled models e.g., in the piezoelectricity and in the fluid-structure interaction. One of the results of such an analysis is the derivation of an approximation of solutions to the complex (complicated) PDE's models by means of solutions to simpler PDE's models in geometrical domains which are more *attractive* e.g., from numerical point of view. For mathematical and numerical analysis of optimization and inverse problems the asymptotic analysis furnishes the possibility to include some singular variations of shapes with the real simplification of numerical procedures which is now documented e.g., in the optimal design of structural mechanics by wide application of the so-called topological derivatives of shape functionals. Therefore, it seems to be important for the applications in real world problems and numerical solution of optimization

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problems to have in hand the applied asymptotic analysis of mathematical models including the formulae which can be really used in modeling and computations. We restrict ourselves to the elastic bodies and we assemble the results for the so-called polarization matrices in elasticity, it is the first paper on the subject in this setting.

1.1. Motivation. Any asymptotic (approximative) formula for the stress-strain state of an elastic body with small, sparsely placed defects includes the so-called defect polarization matrices. Such matrices are generalizations of classical objects in harmonic analysis, namely quadratic forms associated to polarization tensors and virtual masses (see [53]). Apparently these integral attributes were introduced and analyzed in the context of three and two dimensional isotropic elasticity theory in [34, 35], where polarization matrices were used in the asymptotic analysis of the stress-strain state of a defected solid. Polarization matrices are employed to describe asymptotic properties of elastic bodies with small inclusions, holes or cavities, voids and cracks, also in anisotropic elastic materials [44]. There are generalizations of this concept, see e.g. [42, 51] and also [[49]; Chapter 5] where analogous matrices are defined for more general elliptic systems. We also refer to the books [13, 4, 3]where the polarization matrices and tensors are analyzed and applied from physical and numerical points of view. In the present papers, the authors present a rigorous introduction to the field of polarization objects in elasticity in two and three spatial dimensions, the generic properties of such objects are investigated and the shape sensitivity analysis is performed.

We start with the simplest examples.

1.2. Simple formulae in the two-dimensional case. Let  $\omega$  be a domain in the plane  $\mathbb{R}^2$  with compact closure  $\overline{\omega} = \partial \omega \cup \omega$ . We assume the boundary  $\partial \omega$ as piecewise smooth with a finite collection  $\mathcal{Q} = \{\mathcal{O}^1, \ldots, \mathcal{O}^N\}$  of angular points  $\mathcal{O}^j$  with opening angles  $\alpha_q \in (0, 2\pi]$ . The origin  $\mathcal{O} := \{x = 0\}$  of the Cartesian coordinate system is situated in the interior of  $\omega$ . We consider the solutions  $z^j$  of the exterior Neumann problem for the Laplace equation

(1.1) 
$$-\Delta z^j(x) = 0$$
,  $x \in \Omega := \mathbb{R}^2 \setminus \overline{\omega}$ ,  $\partial_n z^j(x) = -n_j(x)$ ,  $x \in \partial \omega \setminus \mathcal{Q}$ ,

where  $n = (n_1, n_2)$  is the unit outward normal to the boundary  $\partial \Omega$  of  $\Omega$ , determined everywhere on  $\partial \omega$  except at the angular points  $\mathcal{O}^j$ , and  $\partial_n$  stands for the normal derivative. If we require in addition that  $z^j$  decays at infinity the evident identities

(1.2) 
$$\int_{\partial \omega} n_j(x) ds_x = 0 , \quad j = 1, 2,$$

ensure the existence of the unique solutions  $z^j$  to problem (1.1). Moreover, the solutions admit the asymptotic representation

$$z^{j}(x) = \sum_{k=1}^{2} m_{jk} \frac{\partial f}{\partial x_{k}}(x) + O(|x|^{-2}) = -\frac{1}{2\pi} \sum_{k=1}^{2} m_{jk} \frac{x_{j}}{|x|^{2}} + O(|x|^{-2}) , \quad |x| > R,$$

where  $f(x) = -(2\pi)^{-1} \ln |x|$  is the fundamental solution of the Laplacian in  $\mathbb{R}^2$ ,  $f^j(x) = -(2\pi |x|^2)^{-1} x_j$  are its derivatives and the radius R is chosen such that  $\overline{\omega}$  belongs to the circle  $\{x : |x| < R\}$ . Formula (1.3) can be differentiated with the convention

(1.4) 
$$\nabla O(|x|^{-\tau}) = O(|x|^{-\tau-1}) \; .$$

The coefficients  $m_{jk}$  in (1.3) give rise to a  $2 \times 2$  matrix  $m = m(\omega)$  which defines one of the classical integral characteristics of the domain  $\omega$  in the harmonic analysis, namely, the matrix associated with the virtual mass tensor of the set  $\overline{\omega}$  (see [[53]; Appendix G]). It is symmetric and negative definite in the case  $mes_2(\omega) > 0$ ).

For a circle  $\omega = \{x : |x| < R\}$  of radius R > 0, we have  $n(x) = -R^{-1}x$ ,  $\partial_n = -\partial/\partial |x|, z^j(x) = R^2 |x|^{-2} x_j$  and, thus

(1.5) 
$$m = -2\pi R^2 \mathbb{I}_2$$
,

where for  $N \in \mathbb{N}$ ,  $\mathbb{I}_N$  is the unit matrix of size  $N \times N$ .

Now let us consider the analogous boundary value problem for the homogeneous isotropic elastic plane with the hole  $\overline{\omega}$ . The system of equilibrium equations

(1.6) 
$$-\mu\Delta z_k - (\lambda + \mu)\frac{\partial}{\partial x_k} \left(\frac{\partial z_1}{\partial x_1} + \frac{\partial z_2}{\partial x_2}\right) = 0 \quad \text{in} \quad \Omega \ , \quad k = 1, 2 \ ,$$

together with the boundary conditions

(1.7) 
$$\sigma_k^{(n)}(z) = g_k \quad \text{on} \quad \partial \omega , \quad k = 1, 2 ,$$

contain the Lamé constants  $\lambda \ge 0$  and  $\mu > 0$  of the elastic material, the displacement vector z with the projections  $z_k$  on the  $x_k$ -axes and the traction components

(1.8) 
$$\sigma_k^{(n)}(z) = n_1 \sigma_{1k}(z) + n_2 \sigma_{2k}(z) , \quad k = 1, 2 .$$

The Cartesian components  $\sigma_{jk}(z)$  of the stress tensor  $\sigma(z)$  of rank 2 are given by the Hooke's law

(1.9) 
$$\sigma_{jk}(z) = 2\mu\varepsilon_{jk}(z) + \lambda\delta_{j,k}(\varepsilon_{11}(z) + \varepsilon_{22}(z)) ,$$

where  $\delta_{j,k}$  stands for Kronecker's symbol and

(1.10) 
$$\varepsilon_{jk}(z) = \frac{1}{2} \left( \frac{\partial z_j}{\partial x_k} + \frac{\partial z_k}{\partial x_j} \right), \quad j = 1, 2,$$

are Cartesian components of the strain tensor  $\varepsilon(z)$ .

The special displacement vectors

(1.11) 
$$\mathbf{D}^{11}(x) = (x_1, 0)$$
,  $\mathbf{D}^{22}(x) = (0, x_2)$ ,  $\mathbf{D}^{12}(x) = \mathbf{D}^{21}(x) = (x_2, x_1)$ ,

enjoy the property

(1.12) 
$$\varepsilon_{jk}(\mathbf{D}^{pq};x) = \delta_{j,p}\delta_{q,k} , \quad j,k,p,q = 1,2.$$

Let  $\mathbf{Z}^{pq}$  denote solutions of the exterior elasticity problem (1.6), (1.7) with the right-hand sides

(1.13) 
$$g_k := -\sigma_k^{(n)}(\mathbf{D}^{pq}) = -2\mu\delta_{k,q}n_p - \lambda\delta_{p,q}n_k , \quad k = 1, 2,$$

calculated according to formulae (1.9)-(1.12). In view of (1.2), functions (1.13) have zero mean value over  $\partial \omega$ . Hence, problem (1.6), (1.7), (1.13) admits a unique solution decaying at infinity.

We recall the fundamental solution matrix for the elliptic  $(2 \times 2)$ -matrix  $L(\nabla_x)$  of differential operators in the left-side of (1.6), the so-called Somigliana tensor

(1.14) 
$$F(x) = (F^1(x), F^2(x))$$

$$=\frac{1}{8\pi\mu(\lambda+2\mu)} \begin{bmatrix} -2(\lambda+3\mu)\ln|x|+2(\lambda+\mu)x_1^2|x|^{-2} & 2(\lambda+\mu)x_1x_2|x|^{-2}\\ 2(\lambda+\mu)x_1x_2|x|^{-2} & -2(\lambda+3\mu)\ln|x|+2(\lambda+\mu)x_2^2|x|^{-2} \end{bmatrix}$$

Near infinity, the solutions  $\mathbf{Z}^{pq}$  can be decomposed into linear combinations of derivatives of the columns  $F^1$  and  $F^2$  in (1.14). Recalling convention (1.4), we introduce the first order decomposition

(1.15) 
$$\mathbf{Z}^{pq}(x) = \sum_{j,k=1}^{2} \mathbf{P}_{jk}^{pq} F^{jk}(x) + O(|x|^{-2}),$$

where

(1.16) 
$$F^{jk}(x) = D_1^{jk}(\nabla)F^1(x) + D_2^{jk}(\nabla)F^2(x), \text{ i.e.}$$
$$F^{11} = \frac{\partial}{\partial x_1}F^1, \quad F^{22} = \frac{\partial}{\partial x_2}F^2, \quad F^{12} = F^{21} = \frac{\partial}{\partial x_2}F^1 + \frac{\partial}{\partial x_1}F^2.$$

We emphasize that the right-hand side of (1.15) contains all first order derivatives of  $F^1$  and  $F^2$  with exception of  $\frac{\partial}{\partial x_2}F^1 - \frac{\partial}{\partial x_1}$ . As it can be seen by the same arguments as in Lemma 2.5 below, this term is absent in (1.15) due to the identity

$$\int_{\partial\omega} (n_1(x)x_2 - n_2(x)x_1)ds_x = 0.$$

The coefficients  $\mathbf{P}_{jk}^{pq}$  in (1.15) give rise to a symmetric, negative definite tensor  $\mathbf{P}$  of rank 4 which is called the polarization tensor of the cavity  $\overline{\omega}$  in the isotropic plane (see [35])

**Remark 1.1.** The polarization matrices for the circle can be calculated explicitly, see [11], e.g. In crack theory this integral characteristic is related to the Neumann problem in  $\mathbb{R}^2 \setminus (\Lambda \cup \Upsilon)$ , where  $\Lambda$  is the semiinfinite crack  $\{(x_1, 0) : x_1 < 0\}$  and  $\Upsilon$ is a crack shoot  $\Upsilon = \{(x_1, f(x_1)) : x_1 \in [0, h)\}$  with a fixed h > 0, and a smooth function f. It is well known that there exist two linear independent solutions to the homogeneous elasticity problem with homogenous Neumann boundary conditions in the domain  $\mathbb{R}^2 \setminus \Lambda$  which grow like  $|x|^{1/2}$  as  $|x| \to \infty$ , they play the role of the coordinate-functions  $x_j$  in (1.1). Correspondingly there appear two solutions  $\sim |x|^{-1/2}$  in the asymptotics of solutions with finite elastic energy on the domain  $\mathbb{R}^2 \setminus (\Lambda \cup \Upsilon)$ , their coefficients give rise to the Polarization matrix in this case.

1.3. State of art and preliminaries. The main applications for polarization matrices (tensors) can be listed as follows

- problems of damage and fracture;
- mechanics of composites, especially dilute composites, i.e., with sparsely distributed defects and inclusions;
- vibration of inhomogeneous bodies;
- shape optimization

For the first topic we refer to the classical paper of Griffith [12] which is in fact devoted to the evaluation of the polarization matrix for a crack located in the isotropic plane. Actually the matrix enters asymptotic formulae for the variation of energy of deformation which govern the nucleation or the growth for a straight crack (cf. [24]). There are many papers on similar problems in three spatial dimensions, and also on a description of interactions between a main crack with some defects of different nature (see e.g., the papers [34, 31, 32, 33, 45] and the books [19, 23, 28]). We point out, that curving and kinking of cracks is described by matrices which are fully analogous to the polarization matrices (cf. [50, 6, 40]).

For the second topic, polarization tensors are also useful tools in analysis and description of effective properties of dilute composites, which leads to approximate but explicit formulae (see books [13, 2, 28, 30], and papers [41, 6, 8]). This is also the way to obtain the mathematical definitions of damage tensors and measures (cf. [44, 46, 47]).

Concerning the third topic, we mention that in spectral problems with small singular perturbations of the boundary the leading term in the asymptotics of the eigenvalues can be calculated as a function of the polarization matrix or similar objects (see the papers [25, 9, 10, 52] and the books [23], [28]<sup>1</sup>)

In shape optimization the polarization matrices are one of the main ingredients of the topological derivatives of shape functionals [51], even if it is not explicitly acknowledged. The integral attributes of inclusions can be identified also in terms of the polarization matrices [4, 3]. In particular, in shape optimization and identification problems for eigenvalues, the role of polarization matrices seems to be premondial [52, 39].

Evidently, the polarization matrices (tensors) are quite important for modeling in solid mechanics. Unfortunately, the matrices are known explicitly only for some specific canonical shapes, e.g. among others for a ball and an ellipse, for an elliptic plane crack in three spatial dimensions and a straight crack in two spatial dimensions. The famous theorem of Eshelby on elliptic inclusions ([11, 13] and others) provides simple but implicit algebraic formulae, with broad applications in the literature in mechanics. We indicate the close connection of the polarization matrices to the Eshelby theorem in Section 2.6

Let us point out that the results presented in [26, 27] and reproduced in [28] on the explicit representations of polarization matrices for arbitrary shaped cavities in the isotropic plane, are wrong. A mistake is found and is discussed in [5], however, after correction the problem reduces to solving an infinite system of algebraic equations and then, sadly enough, makes the correct formulae completely implicit.

In three dimensional elasticity, there are no general constructive results on the evaluation of polarization matrices. The difficulty arises since it is necessary to solve a transmission problem in unbounded domains which makes it impossible to apply the standard numerical schemes usually designed for bounded domains.

The plan of this paper is as follows: In section 1.4 we give a short recapitulation of the results for the two dimensional exterior Neumann problem in isotropic elasticity. In Section 2 of the present paper we investigate the polarization matrices in elasticity in three spatial dimensions, most of the attention is paid to describe the matrices in the form of intrinsic integral and energy attributes of cavities and elastic or rigid inclusions. Such representations provide a description of general properties, e.g., positiveness/negativeness (see Theorems 2.7 and 2.8) and are very useful in the shape sensitivity analysis of Section 3.

We use the matrix/column notation for constitutive laws in elasticity (see [20, 49]) which is described in Section 1.4. Note that the concept of algebraically equivalent media (cf. [7, 14] for two dimensional case and [17, 18] for three dimensions) allows for simple formulae of the entries of polarization matrices, but only in the case of very specific shapes and stiffness tensors (see Section 2.5).

In section 3 we perform the shape sensitivity analysis of polarization matrices. The benefits of these results are twofold. First, if the polarization matrix is known

<sup>&</sup>lt;sup>1</sup>In paper [27] there is an error which is repeated in [28] and it is corrected in [10].

for a specific shape, we can use the shape derivatives in order to evaluate the matrix for a regular perturbation of the shape. The second application concerns the shape optimization, identification and design in structural mechanics. We can minimize/maximize a specific functional with respect to the polarization matrices, some applications in inverse problems can be found e.g. in [3], but it is still the field of current research. There are at least two possible approaches to the shape sensitivity analysis. One is based on the asymptotic analysis in singularly perturbed domains, the method is explained in details for the elasticity in two dimensions. The second method uses the boundary variation technique [55] for the shape functionals which resemble the energy functionals. In this way we derive directly the shape derivatives of the polarization matrices written in the form of a minimizer of the given functional, or, equivalently, evaluate the material derivatives of the minimizers and obtain the same expression for the shape derivatives of the polarization matrices. In any case our analysis deals with elliptic boundary value problems in unbounded domains and requires the appropriate technique of Kondratiev spaces.

1.4. The matrix/column notation and the polarization matrix for two dimensional elasticity problems. Let us fix the Cartesian coordinate system  $x = (x_1, x_2)^{\top}$  and consider the displacement vector z as a column  $z = (z_1, z_2)^{\top} \in \mathbb{R}^2$ , here  $^{\top}$  denotes transposition. We arrange strains and stresses in columns are of height 3 :

(1.17) 
$$\begin{aligned} \varepsilon(u) &= (\varepsilon_{11}(u), \varepsilon_{22}(u), \sqrt{2\varepsilon_{12}(u)})^{\top} \\ \sigma(u) &= (\sigma_{11}(u), \sigma_{22}(u), \sqrt{2\sigma_{12}(u)})^{\top} \end{aligned}$$

The factor  $\sqrt{2}$  is used in the last components of the columns in order to keep the same euklidian norms for the tensor and its representation in the form (1.17). In particular, in thereby ensure, (see [43] and e.g., [49]) that the orthogonal transformations  $x \mapsto \theta x$  and  $z \mapsto \theta z$  induce the orthogonal transformations  $\varepsilon \mapsto \Theta \varepsilon$  and  $\sigma \mapsto \Theta \sigma$  of the corresponding columns given in (1.17). Here, by  $\theta$  and  $\Theta$  we denote orthogonal matrices of size (2 × 2) and (3 × 3), respectively,

$$\theta = \begin{bmatrix} \cos\vartheta & \sin\vartheta \\ -\sin\vartheta & \cos\vartheta \end{bmatrix}, \quad \Theta = \begin{bmatrix} \cos^2\vartheta & \sin^2\vartheta & -2^{-1/2}\sin 2\vartheta \\ \sin^2\vartheta & \cos^2\vartheta & 2^{-1/2}\sin 2\vartheta \\ 2^{-1/2}\sin 2\vartheta & -2^{-1/2}\sin 2\vartheta & \cos 2\vartheta \end{bmatrix}.$$

Hooke's law (1.9) reduces to the form

(1.19) 
$$\sigma(u) = A\varepsilon(u) , \quad \text{where } A = \begin{bmatrix} \lambda + 2\mu & \lambda & 0\\ \lambda & \lambda + 2\mu & 0\\ 0 & 0 & 2\mu \end{bmatrix} .$$

This matrix serves for the homogeneous and isotropic material with Lamé constants  $\lambda$  and  $\mu$ , while for an inhomogeneous and anisotropic body the matrix A in relation (1.19) can be an arbitrarily symmetric and positive definite  $(3 \times 3)$ -matrix function. Clearly, in the isotropic homogeneous case, the matrix A satisfies the identity  $A = \Theta^{\top}A\Theta$  for any  $\vartheta \in [0, 2\pi)$ , however, this transformation changes an anisotropic stiffness matrix although preserving its general properties.

Owing to (1.10) and (1.17), the strain column takes the form

(1.20) 
$$\varepsilon(z;x) = D(\nabla)z(x)$$

(1.21) 
$$D(\xi) = \begin{bmatrix} \xi_1 & 0\\ 0 & \xi_2\\ 2^{-1/2}\xi_2 & 2^{-1/2}\xi_1 \end{bmatrix}, \quad \xi = \begin{bmatrix} \xi_1\\ \xi_2 \end{bmatrix}.$$

Finally, problem (1.6), (1.7) in the matrix notation reads

(1.22) 
$$D(-\nabla)^{\top}AD(\nabla)z(x) = 0, \quad x \in \Omega, \\ D(n(x))^{\top}AD(\nabla)z(x) = g(x), \quad x \in \partial\Omega$$

The elasticity problem in the divergence form (1.22) mimics the Neumann problem for a formally self-adjoint second-order elliptic operator and it is very convenient for standard manupulations. Bulking (see formula (1.24) below) occurs only in rewriting expansion (1.15) with the polarization matrix of the size  $(3 \times 3)$ .

The polarization matrix  $P = (P_{pq})_{p,q=1}^3$  can be reconstructed from the polarization tensor **P** as follows

(1.23) 
$$P_{11} = \mathbf{P}_{11}^{11} , \quad P_{22} = \mathbf{P}_{22}^{22} , \quad P_{33} = \mathbf{P}_{12}^{12} , \\ P_{13} = \sqrt{2}\mathbf{P}_{12}^{11} , \quad P_{23} = \sqrt{2}\mathbf{P}_{12}^{22} .$$

Recall that the symmetry of the rank 4 tensor **P** means that  $\mathbf{P}_{jk}^{pq} = \mathbf{P}_{jk}^{qp} = \mathbf{P}_{pq}^{qp}$  for any j, k, p, q = 1, 2 while for the symmetric matrix P we have  $P_{jk} = P_{kj}$ . Note that the vectors (1.11) are of similar type as the rows  $D^1(x), D^2(x), D^3(x)$ 

Note that the vectors (1.11) are of similar type as the rows  $D^1(x)$ ,  $D^2(x)$ ,  $D^3(x)$  of the matrix D(x), while relations (1.12) turn into  $D(\nabla)D(x)^{\top} = \mathbb{I}_{3\times 3}$ . By  $Z^p$  we denote solutions of the exterior elasticity problem (1.22) with  $g = -D(n)^{\top}A\mathbf{e}_p$  where p = 1, 2, 3 and  $\mathbf{e}_p = (\delta_{1,p}, \delta_{2,p}, \delta_{3,p}) \in \mathbb{R}^3$ .

It is useful to introduce the  $(2 \times 3)$ -matrix  $Z = (Z^1, Z^2, Z^3)$  which satisfies the *matrix* variant of problem (1.22) where now the right-hand side  $g = -D(n)^{\top}A$  is a matrix of size  $2 \times 3$ . In view of (1.23), expansions (1.15) convert into the relations

$$Z^{p}(x) = \sum_{q=1}^{3} P_{pq} D^{q}(\nabla)^{\top} F(x) + O(|x|^{-2}) , \quad p = 1, 2, 3,$$

which results in the formula

(1.24) 
$$Z(x) = (D(\nabla)F(x)^{\top})^{\top}P + O(|x|^{-2}) .$$

This funny way of writing (cf. (2.40) below) occurs because it is necessary to put differentiation and multiplication in a correct order.

**Remark 1.2.** The tensor nature of the object of the object  $\mathbf{P} = \mathbf{P}(\omega)$  can be seen by the following observation. If  $\Xi \subset \mathbb{R}^2$  is a smoothly surrounded domain and  $\omega_h = \{x : h^{-1}x \in \omega\}$  a small hole of diameter  $h \ll 1$ , then the corresponding potential energy  $U^h$  of the body  $\Xi \setminus \overline{\omega}_h$  can be calculated asymptotically to

(1.25) 
$$U^{h} = U^{0} - \frac{1}{2}h^{2}\sum_{j,k=1}^{2}\sum_{p,q=1}^{2}\varepsilon_{jk}(u;0)\mathbf{P}_{pq}^{jk}\varepsilon_{pq}(u;0) + O(h^{3})$$
$$= U^{0} - \frac{1}{2}h^{2}\varepsilon(u;0)^{\top}P(\omega)\varepsilon(u;0) + O(h^{3})$$

(cf. [24, 34, 51]), where u and  $U^0$  denote the displacement field and potential energy in the entire elastic body  $\Xi$ . Since  $U^h$  is a scalar and  $\varepsilon(u)$  is a tensor of rank 2, necessarily  $\mathbf{P}(\omega)$  is a tensor of rank 4.

**Remark 1.3.** Formulae (1.5) together with (1.23) show that the polarization tensors (matrices) depend quadratically on the diameter of the hole  $\overline{\omega} \subset \mathbb{R}^2$ . This is a common property of the two-dimensional case namely that  $\mathbf{P}(\omega_h) = h^2 \mathbf{P}(\omega)$  and the energy increment can be evaluated as follows

$$U^h - U^0 \approx -\frac{1}{2}\varepsilon(u;0)P(\omega_h)\varepsilon(u;0)$$
.

For the three-dimensional case the analogous formula  $P(\omega_h) = h^3 P(\omega)$  is verified in (2.51).

### 2. The polarization matrices for three-dimensional anisotropic elasticity problems

2.1. The mathematical setting as an exterior boundary value problem. As already mentioned, we need solutions of various exterior boundary value problems. We start with introducing some geometrical notations. The ball and the sphere of radius R > 0 are denoted by  $\mathbb{B}_R$  and  $\mathbb{S}_R$ , respectively. Let  $\Omega \subset \mathbb{R}^3$  be a Lipschitz domain with a compact connected complement  $\Omega^{\bullet}$  and boundary  $\Gamma$ . For  $x \in \Gamma$ , we denote by n(x) the outward (with respect to  $\Omega$ ) unit normal vector. For integer l,  $H^l(\Omega)$ ,  $H^l(\Omega^{\bullet})$  and - in case of smooth  $\Gamma$  – the spaces  $H^s(\Gamma)$  for  $s \in \mathbb{R}$  are the usual Sobolev-Slobodetskii spaces (see [21], e.g.) If  $\Gamma$  is only Lipschitz, then at least the trace space  $H^{1/2}(\Gamma)$  is well defined together with a continuous trace operator  $\gamma : H^1(\Omega^{\bullet}) \to H^{1/2}(\Gamma)$ , such that  $\gamma \phi = \phi|_{\Gamma}$  for smooth functions. We keep the notation  $\phi|_{\Gamma}$  also for  $H^1$ -functions. The trace operator possesses a continuous right inverse: For  $\phi \in H^{1/2}(\Gamma)$  there exists  $\Phi^{\bullet} \in H^1(\Omega^{\bullet})$  such that  $\Phi^{\bullet}|_{\gamma} = \phi$  and

(2.1) 
$$\|\Phi^{\bullet}; H^{1}(\Omega^{\bullet})\| \leq C(\Gamma) \|\phi; H^{1/2}(\Gamma)\|$$

Similar as in section 1.4, we think of the displacement vector  $u = (u_1, u_2, u_3)^{\top}$  as a column in  $\mathbb{R}^3$  and introduce the strain column of height 6

(2.2) 
$$\varepsilon(u) = (\varepsilon_{11}(u), \varepsilon_{22}(u), \varepsilon_{33}(u), \alpha^{-1}\varepsilon_{23}(u), \alpha^{-1}\varepsilon_{31}(u), \alpha^{-1}\varepsilon_{12}(u))^{\top}$$

where  $\alpha = 2^{-1/2}$  and again,  $\varepsilon_{jk}(u)$  are Cartesian components of the strain tensor given by (1.10) with j, k = 1, 2, 3. Like in (1.20), (1.21), we have

$$\varepsilon(u) = D(\nabla)u,$$

(2.3) 
$$D(\xi)^{\top} = \begin{pmatrix} \xi_1 & 0 & 0 & \alpha \xi_3 & \alpha \xi_2 \\ 0 & \xi_2 & 0 & \alpha \xi_3 & 0 & \alpha \xi_1 \\ 0 & 0 & \xi_3 & \alpha \xi_2 & \alpha \xi_1 & 0 \end{pmatrix}, \qquad \xi \in \mathbb{R}^3.$$

Analogously to (2.2), we define the stress columns  $\sigma(u)$  and  $\sigma^{\bullet}(u)$  in  $\Omega$  and  $\Omega^{\bullet}$ , respectively,

(2.4) 
$$\sigma(u) = A\varepsilon(u), \qquad \sigma^{\bullet}(u) = A^{\bullet}\varepsilon(u).$$

Here A and  $A^{\bullet}$  are symmetric and positive definite  $6 \times 6$  matrices containing the elastic moduli of the material. We assume that the matrix A has the form  $A(x) = A^0 + A^e(x)$ , where entries of  $A^e$  are  $C^1$ -functions on  $\overline{\Omega}$  with  $A^e(x) = 0$  for r = |x| large, say  $r \geq R_0$ . We also assume that  $R_0$  large enough such that  $\overline{\Omega^{\bullet}}$  is contained

in the open ball  $\mathbb{B}_{R_0}$ . The matrix  $A^0$  is constant and positive definite, i.e. the elastic space is homogeneous far away from the inclusion. However, the inclusion again can be heterogeneous, we suppose that the entries of  $A^{\bullet}$  are  $C^1$ - functions in  $\overline{\Omega^{\bullet}}$ , e.g.. Both the matrices A(x) and  $A^{\bullet}(x)$  must be uniformly positive definite, i.e.

(2.5) 
$$\xi^{\top} A(x)\xi \ge a|\xi|^2 , \quad \xi^{\top} A^{\bullet}(x)\xi \ge a_{\bullet}|\xi|^2$$

holds for any vector  $\xi \in \mathbb{R}^6$  and all  $x \in \Omega$  and  $x \in \Omega^{\bullet}$  with positive constants  $a, a_{\bullet}$ . The elasticity problem in  $\Omega \cup \Omega^{\bullet}$  reads as follows:

(2.6) 
$$D(-\nabla)^{\top}A(x)D(\nabla)u(x) = f(x), \qquad x \in \Omega = \mathbb{R}^3 \setminus \overline{\Omega^{\bullet}}; \\ D(-\nabla)^{\top}A^{\bullet}(x)D(\nabla)u^{\bullet}(x) = f^{\bullet}(x), \qquad x \in \Omega^{\bullet};$$

$$\begin{array}{lll} & u(x) - u^{\bullet}(x) &=& g^{0}(x), \\ D(n(x))^{\top} A(x) D(\nabla) u(x) - D(n(x))^{\top} A^{\bullet}(x) D(\nabla) u^{\bullet}(x) &=& g^{1}(x), \\ (2.8) & |u(x)| = O(|x|^{-1}), & \text{as } |x| \to \infty. \end{array}$$

Here f,  $f^{\bullet}$  are volume forces while  $g^0$  and  $g^1$  stand for jumps of displacements and tractions on the interface  $\Gamma$ . To shorten the notations, we denote the differential operators (2.6) by  $\mathcal{L}$  and  $\mathcal{L}^{\bullet}$  respectively; similarly, we express the left-hand side of (2.7)<sub>1</sub> as:  $\mathcal{N}u - \mathcal{N}^{\bullet}u^{\bullet}$ .

We look for a variational formulation of this problem. By  $\mathcal{H}$ , we denote the completion of  $C_0^{\infty}(\mathbb{R}^3)^3$  with respect to the "energy" norm

$$||D(\nabla)u;L^2(\mathbb{R}^3)||.$$

Using the Fourier transform and Hardy's inequality, we obtain the Korn's inequality

$$(2.10) \ \|(1+r)^{-1}u; L^2(\mathbb{R}^3)\| + \|\nabla u; L^2(\mathbb{R}^3)\| \leqslant \frac{1}{\sqrt{10}} \|D(\nabla)u; L^2(\mathbb{R}^3)\| \qquad u \in \mathcal{H}.$$

In this context we recall the definition of Kondratiev norms, adapted to the special cases we need here: Let  $G \subseteq \mathbb{R}^3$  an (unbounded) domain,  $\beta \in \mathbb{R}$  and  $l \in \mathbb{N}_0 = \{0, 1, \ldots\}$  be fixed. Then the Kondratiev space  $V^l_\beta(G)$  consists of all  $u \in H^l_{loc}(\overline{G})$  such that the norm

$$\|u; V_{\beta}^{l}(G)\| = \left(\sum_{k=0}^{l} \|(1+|x|)^{\beta-l+k} \nabla_{x}^{k} u; L^{2}(G)\|^{2}\right)^{1/2} < \infty.$$

Note that the weight control the behavior at infinity of the functions under consideration. Estimate (2.10) implies that  $\mathcal{H} = V_0^1(\mathbb{R}^3)$  and the norms are equivalent.

In the sequel we use the notation  $(,)_{\Xi}$  for the scalar product in  $L^2(\Xi)$  for various suitable sets  $\Xi \subset \mathbb{R}^3$ . For sufficiently smooth vector fields u and v we have Green's formulae on  $\Omega$  and  $\Omega^{\bullet}$ :

(2.11) 
$$(\mathcal{L}u, v)_{\Omega} + (\mathcal{N}u, v)_{\Gamma} = (AD(\nabla)u, D(\nabla)v)_{\Omega},$$

(2.12) 
$$(\mathcal{L}^{\bullet}u, v)_{\Omega} - (\mathcal{N}^{\bullet}u, v)_{\Gamma} = (A^{\bullet}D(\nabla)u, D(\nabla)v)_{\Omega^{\bullet}}.$$

Note that n is the *internal* normal vector on  $\Gamma$  with respect to  $\Omega^{\bullet}$ . That is why there appears the sign minus in (2.12). In particular, for any vector function  $u \in H^2_{loc}(\overline{\Omega})$ ,

 $u^{\bullet} \in H^2(\Omega^{\bullet})$ , satisfying (2.6) and (2.7), and  $v \in C_0^{\infty}(\mathbb{R}^3)$ , the addition of the two formulae leads to

(2.13)

$$(AD(\nabla)u, D(\nabla)v)_{\Omega} + (A^{\bullet}D(\nabla)u^{\bullet}, D(\nabla)v)_{\Omega^{\bullet}} = (f^{\bullet}, v)_{\Omega^{\bullet}} + (f, v)_{\Omega} + (g^{1}, v)_{\Gamma}$$

If  $g^0 = 0$  and  $u \in V_1^2(\Omega)$  in the situation above, then we can glue  $u, u^{\bullet}$  together and obtain a vector field  $w \in V_0^1(\mathbb{R}^3) = \mathcal{H}$ . Furthermore, due to our assumptions on the matrices  $A, A^{\bullet}$  and Korn's inequality (2.10), the left hand side of this equality defines a scalar-product  $\mathbf{b}(, )$  on  $\mathcal{H}$  which induces a norm equivalent to the energy norm defined by (2.9). If f and  $f^{\bullet}$  are restrictions of  $F \in V_1^0(\Omega)$  the right hand side of (2.13) defines a continuous linear functional on  $\mathcal{H}$ , even in case  $(g^1, v)_{\Gamma}$  being replaced by  $\langle g^1, v \rangle$  with  $g^1 \in H^{-1/2}(\Gamma)$ . Thus, for  $g^0 = 0$ , equation (2.13) takes the form

(2.14) 
$$\mathbf{b}(u,v) = \mathscr{F}(v) \text{ with } \mathscr{F} \in \mathcal{H}'$$

Clearly, Neumann boundary values in general do not exist for  $u \in \mathcal{H}$ . Since  $\mathcal{L}, \mathcal{L}^{\bullet}$  are differential operators in divergence form, we may use a well known weak trace theorem to overcome this difficulty (see [56, Lemma ?]).

**Proposition 2.1.** For  $u \in H^1(\Omega^{\bullet})^3$  with  $\mathcal{L}^{\bullet} u \in L^2(\Omega)^3$ , there exists a trace  $\mathcal{N}^{\bullet} u \in H^{-1/2}(\Gamma)$ , such the Green's formula (2.12) is valid and the following estimate holds independent of u:

(2.15) 
$$\|\mathcal{N}^{\bullet}u; H^{-1/2}(\Gamma)\| \leq C \left(\|D(\nabla)u; L^{2}(\Omega)\| + \|\mathcal{L}^{\bullet}u; L^{2}(\Omega)\|\right).$$

An analogous result is true for  $u \in V_0^1(\Omega)$  with  $\mathcal{L}u \in V_1^0(\Omega)$ .

To rewrite the general problem (2.6) - (2.8) in the form (2.14), it is necessary to reduce it to the case  $g^0 = 0$ . The obvious way is here to search for  $u^{\bullet} = U^{\bullet} - G$ , where G is a suitable extension of  $g^0$  onto  $\Omega^{\bullet}$ . If  $g^0 \in H^{3/2}(\Gamma)$ , this works with any extension  $G \in H^2(\Omega^{\bullet})$ . For  $g^0 \in H^{1/2}$  we take the unique weak solution  $G \in H^1(\Omega)$ to the problem

(2.16) 
$$\mathcal{L}^{\bullet}G = 0 \quad \text{in } \Omega^{\bullet}, \qquad G = g^0 \quad \text{on } \Gamma$$

Here we have the estimate

(2.17) 
$$||G; H^1(\Omega^{\bullet})|| \leq C ||g^0; H^{1/2}(\Gamma)|$$

with a constant independent of  $u^0$ , and by regularity results for elliptic problems [57] this extends to

(2.18) 
$$||G; H^{l+2}(\Omega^{\bullet})|| \leq C ||g^0; H^{l+3/2}(\Gamma)||, \quad l \in \mathbb{N}_0,$$

provided the surface  $\Gamma$  as well as the coefficient functions in  $A^{\bullet}$  are sufficiently smooth and  $g^0 \in H^{l+3/2}(\Gamma)$ .

**Definition 2.2.** Let  $f^{\bullet} \in L^2(\Omega^{\bullet})^3$ ,  $f \in V_1^0(\Omega)^3$ ,  $g^0 \in H^{1/2}(\Gamma)$  and  $g^1 \in H^{-1/2}(\Gamma)^3$ be given, and let  $G \in H^1(\Omega^{\bullet})^3$  be the extension of  $g^0$  into  $\Omega^{\bullet}$  defined by (2.16). We call a pair  $\{u, u^{\bullet}\}$  of vector fields defined on  $\Omega$  and  $\Omega^{\bullet}$ , respectively, a weak solution of the boundary value problem (2.6) – (2.8), if  $\{u, u^{\bullet} + G\} \in \mathcal{H}$  and following identity is fulfilled:

$$(2.19) \ (AD(\nabla)u, D(\nabla)v)_{\Omega} + (A^{\bullet}D(\nabla)u^{\bullet}, D(\nabla)v)_{\Omega^{\bullet}} = (f^{\bullet}, v)_{\Omega^{\bullet}} + (f, v)_{\Omega} + \langle g^{1}, v \rangle_{\Gamma}$$

Standard Hilbert space arguments (the Riesz representation theorem) lead to the following result.

**Proposition 2.3.** Problem (2.13) has a unique weak solution, and the following estimate holds:

$$\|u; V_0^1(\Omega)\| + \|u^{\bullet}; H^1(\Omega^{\bullet})\|$$

$$(2.20) \leq c \left( \|f^{\bullet}; L^2(\Omega^{\bullet})\| + \|f; V_1^0(\Omega)\| + \|g^0; H^{1/2}(\Gamma)\| + \|g^1; H^{-1/2}(\Gamma)\| \right)$$

If the surface  $\Gamma$  and the matrix functions A,  $A^{\bullet}$  are smooth and for some  $l \in \mathbb{N} = \{1, 2, ...\}$  we have

(2.21) 
$$\begin{aligned} f \in V_l^{l-1}(\Omega)^3, \quad f^{\bullet} \in H^{l-1}(\Omega^{\bullet})^3, \\ g^0 \in H^{l+1/2}(\Gamma)^3, \quad g^1 \in H^{l-1/2}(\Gamma)^3, \end{aligned}$$

then  $u \in V_l^{l+1}(\Omega)^3$ ,  $u^{\bullet} \in H^{l+1}(\Omega^{\bullet})^3$  and the pair  $\{u, u^{\bullet}\}$  is a strong solution to the elliptic transmission problem (2.6), (2.7). Moreover, the estimate

(2.22) 
$$\|u; V_l^{l+1}(\Omega)\| + \|u^{\bullet}; H^{l+1}(\Omega^{\bullet})\| \leq c\mathfrak{F}_l$$

holds true where  $\mathfrak{F}_l$  denotes the sum of the norms of the data (2.21) in the spaces indicated.

**Proof.** Due to Proposition 2.15 the trace  $\mathcal{N}^{\bullet}G \in H^{-1/2}(\Gamma)$ , and

$$(A^{\bullet}D(\nabla)G, D(\nabla)v)_{\Omega^{\bullet}} + \langle \mathcal{N}^{\bullet}G, v \rangle_{\Gamma} = 0.$$

Thus (2.19) is fulfilled if  $U = \{u, u^{\bullet} + G\}$  solves

(2.23) 
$$\mathbf{b}(U,v) = (f^{\bullet}, v)_{\Omega^{\bullet}} + (f, v)_{\Omega} + \langle g^1 - \mathcal{N}^{\bullet} G, v \rangle_{\Gamma}$$

for all  $v \in \mathcal{H}$ . Clearly, (2.23) is again of the form (2.14), thus application of the Riesz representation theorem for a linear functional in a Hilbert space ensures the existence of a unique solution while estimates (2.10) and (2.17) lead to estimate (2.20). The estimate (2.22) follows then from (2.18) and regularity results for elliptic problems (see, e.g., [54]).

**Remark 2.4.** Of course, equation (2.14) is uniquely solvable for any  $\mathscr{F} \in \mathcal{H}'$ , and we obtain

$$(2.24) ||u;\mathcal{H}|| \leq ||\mathscr{F};\mathcal{H}'||$$

However, for general  $u \in \mathcal{H}$ , the second transmission condition is senseless, and it is obvious that there exist functionals  $\mathscr{F} \in \mathcal{H}$  which are not of the form (2.23) with  $f^{\bullet}$ , f and  $g^{0}, g^{1}$  as in Definition 2.2. At the same time is known that any continuous linear functional on  $V_{0}^{1}(\mathbb{R}^{3})$  has a (non unique) representation as

(2.25) 
$$\mathscr{F}(v) = (f, v)_{\mathbb{R}^3} + \sum_{i=1}^3 (F_i, \partial_i v)_{\mathbb{R}^3},$$

with  $f \in V_1^0(\mathbb{R}^3)$ ,  $F_i \in L^2(\mathbb{R}^3)$ , and

(2.26) 
$$\|\mathscr{F}; V_0^1(\mathbb{R}^3)'\|^2 = \inf\left\{\|f; V_1^0(\mathbb{R}^3)\|^2 + \|F_i; L^2(\mathbb{R}^3)\|^2\right\},$$

where the infimum is taken over all representations. The solution u to (2.14) is independent of f and  $F_i$  appearing in (2.25), of course, as long as they lead to the same functional.

We can introduce a *weak transmission problem*: For given  $\mathscr{F} \in \mathcal{H}', g^0 \in H^{1/2}(\Gamma)$ let G be the solution to (2.16). We call  $\{u, u^{\bullet}\}$  a solution to the weak transmission problem (2.6) and (2.7)<sub>2</sub>, if  $U = \{u, u^{\bullet} + G\} \in \mathcal{H}$  and U solves (2.14). Such a solution always exists and from (2.17), (2.24) and (2.26) we obtain

(2.27) 
$$\begin{aligned} \|u; V_0^1(\Omega)\| + \|u^{\bullet}; H^1(\Omega^{\bullet})\| \\ \leqslant c \left( \|f; V_1^0(\mathbb{R}^3)\| + \sum_i \|F_i; L^2(\mathbb{R}^3)\| + \|g^0; H^{1/2}(\Gamma)\| \right). \end{aligned}$$

Again it is not possible to subtract an arbitrary prolongation  $G \in H^1(\Omega^{\bullet})$  from  $u^{\bullet}$ , since then Green's formula (2.12) leads to a boundary distribution which is contained in  $H^{-3/2}(\Gamma)$  only. Insofar the weak transmission problem is equivalent to find in parallel weak solutions to the problems (2.16) and  $\mathcal{L}u = \mathscr{F}$  in  $\mathbb{R}^3$ , where  $\mathscr{L}$  is the differential operator "glued" together from  $\mathcal{L}^{\bullet}$  and  $\mathcal{L}$ .  $\Box$ 

2.2. Asymptotic behavior of the solutions. For given  $f \in V_{\gamma}^{l-1}(\Omega)$  with  $\gamma \in (l+3/2, l+5/2)$ , let  $\{u, u^{\bullet}\}$  be a weak solution according to Proposition 2.3. Clearly  $V_{\gamma}^{l-1}(\Omega) \subset V_l^{l-1}(\Omega)$  and  $u \in V_l^{l+1}(\Omega)$  then. Since A is constant for  $|x| > R_0$  for a suitable constant  $R_0 > 0$ , we can apply a general result for elliptic boundary values in domains with conical boundary points (see [36, Ch. 6.4], e.g.) to characterize the asymptotic behavior of u at infinity. Thereby, let F denote the fundamental matrix of the differential operator  $L(\nabla)$  in  $\mathbb{R}^3$ , i.e.,

(2.28) 
$$L(\nabla)F(x) = \delta(x)\mathbb{I}_3, \quad x \in \mathbb{R}^3, \quad \text{where } L(\nabla) = D(-\nabla)^\top A^0 D(\nabla)$$

where  $\delta$  is the Dirac measure. Since u can be regarded as a  $V_l^{l+1}$ -solution of an exterior Dirichlet problem in  $\Xi = \{x : |x| > R_0\}$ , we obtain the asymptotic representation for  $|x| > R_0$ 

(2.29) 
$$u(x) = (d(-\nabla)F(x)^{\top})^{\top} a + (D(-\nabla)F(x)^{\top})^{\top} b + \widetilde{u}(x) =: U(x) + \widetilde{u}(x)$$

with  $\widetilde{u} \in V_{\gamma}^{l+1}(\Xi)^3$ . The vectors  $a, b \in \mathbb{R}^6$  are coefficient columns,  $D(\xi)$  is matrix (2.3)<sub>2</sub> and  $d(\xi)$  is a similar matrix (generating the space of rigid motions), defined by

(2.30) 
$$d(\xi)^{\top} = \begin{pmatrix} 1 & 0 & 0 & \alpha\xi_3 & -\alpha\xi_2 \\ 0 & 1 & 0 & -\alpha\xi_3 & 0 & \alpha\xi_1 \\ 0 & 0 & 1 & \alpha\xi_2 & -\alpha\xi_1 & 0 \end{pmatrix}, \quad \alpha = \frac{1}{\sqrt{2}}.$$

If the right hand side f vanishes on  $\Xi$ , then u solves the homogeneous system  $(2.6)_1$  in  $\Xi$ , and due to general results in [22] (see also [36, Ch. 3.6]), the remainder in (2.29) fulfils

(2.31) 
$$|\nabla_x^k \widetilde{u}(x)| \leqslant c_k (1+|x|)^{-3-k}, \quad x \in \Xi, \quad k \in \mathbb{N}_0.$$

We emphasize that the matrices  $(2.3)_2$  and (2.30) satisfy the relations

(2.32) 
$$d(\nabla)d(x)^{\top}\Big|_{x=0} = \mathbb{I}_{6}, \qquad d(\nabla)D(x)^{\top}\Big|_{x=0} = \mathbb{O}_{6}$$
$$D(\nabla)d(x)^{\top} = \mathbb{O}_{6}, \qquad D(\nabla)D(x)^{\top} = \mathbb{I}_{6},$$

where  $\mathbb{O}_N$  is the null matrix of size  $N \times N$ .

**Lemma 2.5.** The coefficient column  $a \in \mathbb{R}^6$  in the representation (2.29) is given by the integral formula

(2.33) 
$$a = \int_{\Omega^{\bullet}} d(x) f^{\bullet}(x) dx + \int_{\Omega} d(x) f(x) dx + \int_{\Gamma} d(x) g^{1}(x) ds_{x}.$$

**Proof.** Let  $\mathcal{X} \in C_0^{\infty}[0,\infty)$  be a cut-off function with  $\mathcal{X}(r) = 1$  for  $r \leq 1$ , and  $\mathcal{X}(r) = 0$  for  $r \geq 2$ . For R > 2, put  $\mathcal{X}_R(x) = \mathcal{X}(|x| - R)$ , then supp  $\mathcal{X}_R \subset \mathbb{B}_{R+2}$ . Let  $\{u, u^{\bullet}\}$  be a weak solution according to Definition 2.2. We use (2.13) with  $v = \mathcal{X}_R d_j$ , where  $d_j$  is the *j*-th row of the matrix *d*, and  $R \geq R_0 + 2$ , so that  $\Omega^{\bullet} \subset \mathbb{B}_{R-2}$ . With (2.32)<sub>3</sub>, we obtain

$$(2.34) \qquad (AD(\nabla)u, D(\nabla)(\mathcal{X}_Rd_j))_{\Omega} = (f^{\bullet}, d_j)_{\Omega^{\bullet}} + (f, \mathcal{X}_Rd_j)_{\Omega} + (g^1, d_j)_{\Gamma}.$$

Again due to  $(2.32)_3$ , we have  $D(\nabla)(\mathcal{X}_R d_j) = -[D(\nabla), \mathcal{X}_R]d_j$ , thus the integrand on the left hand side of (2.34) vanishes outside the annulus  $\{x : R < |x| < R+2\}$ . Moreover we have  $\mathcal{X}_R d_j = d_j$  on the sphere  $\mathbb{S}_R$ , while this expression vanishes on  $\mathbb{S}_{R+2}$ . Thus, integration by parts leads to

$$(AD(\nabla)u, D(\nabla)(\mathcal{X}_Rd_j))_{\Omega} = (AD(\nabla)u, D(\nabla)\mathcal{X}_Rd_j)_{\mathbb{B}_{R+2}\setminus\overline{\mathbb{B}}_R}$$
  
$$= (\mathcal{N}u, \mathcal{X}_Rd_j)_{\partial(\mathbb{B}_{R+2}\setminus\overline{\mathbb{B}}_R)} + (\mathcal{L}u, \mathcal{X}d_j)_{\mathbb{B}_{R+2}\setminus\overline{\mathbb{B}}_R}$$
  
$$= (D(n)^{\top}AD(\nabla)u, d_j)_{\mathbb{S}_R} + (f, \mathcal{X}_Rd_j)_{\mathbb{B}_{R+2}\setminus\overline{\mathbb{B}}_R},$$

where  $n = -R^{-1}x$ , hence we obtain for  $R \ge R_0$ (2.35)

$$(D(n)^{\top}A^{0}D(\nabla)u, d_{j})_{\mathbb{S}_{R}} = (f^{\bullet}, d_{j})_{\Omega^{\bullet}} + (g^{1}, d_{j})_{\Gamma} + (f, \mathcal{X}_{R}d_{j})_{\Omega} - (f, \mathcal{X}_{R}d_{j})_{\mathbb{B}_{R+2}\setminus\overline{\mathbb{B}}_{R}}.$$

Since  $f(1+r)^{5/2} \in L^2(\Omega)$  the integral  $\int_{\Omega} d_j f$  converges and we may pass to the limit  $R \to \infty$  in the right-hand side of (2.35), note that the last integral in (2.35) vanishes then. To calculate the limit of the left-hand side, we insert the asymptotic representation (2.29) of u into (2.35), then by (2.31),  $(D(n)^{\top}AD(\nabla)\tilde{u}, d_j)_{\mathbb{S}_R} = O(R^{-1})$  as  $R \to \infty$ , and we are left with the terms

$$(D(n)^{\top}AD(\nabla)U, d_j)_{\mathbb{S}_R},$$

which can be interpreted as a distribution with compact support applied to the  $C^{\infty}$ -function  $d_j$ . Here we mention that due continuity arguments in spaces of distributions, Green's formula

$$(L(\nabla)\mathfrak{u},\mathfrak{v})_{\mathbb{B}_R} - (\mathfrak{u},L(\nabla)\mathfrak{v})_{\mathbb{B}_R}(D(n)^\top = AD(\nabla)\mathfrak{u},\mathfrak{v})_{\mathbb{S}_R} - (\mathfrak{u},D(n)^\top AD(\nabla)\mathfrak{v})_{\mathbb{S}_R}$$

can be extended from  $\mathfrak{u}, \mathfrak{v} \in C^{\infty}(\mathbb{R}^3)^3$  to  $\mathfrak{u} = \partial^{\alpha} F_k$ , where  $F_k$  is a column of the fundamental solution F. Then the first integral has to be replaced by  $\langle \partial^{\alpha} \delta, \mathfrak{v}_k \rangle = (-1)^{|\alpha|} \partial^{\alpha} \mathfrak{v}_k(0)$ . We apply this argument for  $\mathfrak{u} = U$ , and  $\mathfrak{v} = d_j$ , together with formulae (2.32), this leads to

$$(D(n)^{\top} A D(\nabla) U, d_j)_{\mathbb{S}_R} \langle d(-\nabla)^{\top} a \, \mathbb{I}_3 \delta, d_j \rangle + \langle D(-\nabla)^{\top} b \, \mathbb{I}_3 \delta, d_j \rangle$$
  
=  $(d(\nabla) d_j^{\top}(x) \cdot a + D(\nabla) d_j(x)^{\top} \cdot b) \Big|_{x=0} = a_j.$ 

In order to derive an integral formula for the coefficient vector b in the asymptotic representation (2.29) consider problem (2.6) – (2.8) with the special right-hand sides

(2.36) 
$$\begin{aligned} f^{\bullet}_{(k)}(x) &= D(\nabla)^{\top} A^{\bullet}(x) \mathbf{e}_{(k)}, \qquad f_{(k)}(x) &= D(\nabla)^{\top} A(x) \mathbf{e}_{(k)}, \\ g^{0}_{(k)} &= 0, \qquad \qquad g^{1}_{(k)}(x) &= D(n(x))^{\top} (A^{\bullet}(x) - A) \mathbf{e}_{(k)} \end{aligned}$$

where  $\mathbf{e}_{(k)} = (\delta_{1,k}, \dots, \delta_{6,k})^{\top}$  is the k-th unit vector in  $\mathbb{R}^6$ . Note that  $f_{(k)}$  has a compact support contained in  $\mathbb{B}_{R_0}$  due to the choice of the matrix  $A(x) = A^0 + A^e(x)$ . The data in (2.36) arise if we replace u in the transmission problem (2.6),

(2.7) by the rows of the matrix -D(x). We denote the corresponding unique weak solutions to (2.6) - (2.8) by  $\{Z_{(k)}, Z_{(k)}^{\bullet}\}^2$ . Since

$$\int_{\Omega^{\bullet}} d(x) f^{\bullet}_{(k)}(x) \, dx + \int_{\Omega} d(x) f_{(k)}(x) \, dx + \int_{\Gamma} d(x) g^{1}_{(k)}(x) \, ds_{x} = 0 \in \mathbb{R}^{6} \,,$$

Lemma 2.5 turns the asymptotic form (2.29) for the solution  $Z_{(k)}$  into

(2.37) 
$$Z_{(k)}(x) = (D(\nabla)F(x)^{\top})^{\top}P_{(k)} + \widetilde{Z}_{(k)}(x)$$

where the remainder  $Z_{(k)}$  satisfies (2.31) and  $P_{(k)}(=-b)$  denotes a column of height 6. Regarding  $Z_{(k)}(x)$  as a column for each x, we define the  $3 \times 6$ -matrix  $Z(x) = (Z_{(1)}(x), \ldots, Z_{(6)}(x))$ , and, analogously,  $Z^{\bullet}(x)$ . Hence, due to (2.36) and (2.32), the columns of the matrix

(2.38) 
$$\zeta(x) = D(x)^{\top} + \{Z(x), Z^{\bullet}(x)\}$$

are formal solutions of the homogeneous problem (2.6), (2.7) (as well as the columns of the matrix  $d(x)^{\top}$ ), although they do not belong to the energy space  $\mathcal{H}$ . A slight modification of the proof of Lemma 2.5 (cf. [44, 51]) provides the following assertion.

**Lemma 2.6.** The coefficient column  $b \in \mathbb{R}^6$  in (2.29) is given by the integral formula

(2.39) 
$$b = \int_{\Omega^{\bullet}} \zeta(x)^{\top} f^{\bullet}(x) dx + \int_{\Omega} \zeta(x)^{\top} f(x) dx + \int_{\Gamma} \zeta(x)^{\top} g^{1}(x) ds_{x} - \int_{\Gamma} \left\{ D(n(x))^{\top} A D(\nabla) \zeta(x) \right\}^{\top} g^{0}(x) ds_{x}.$$

2.3. The polarization matrix and its properties. Rewriting the asymptotic representation (2.37) in the condensed form

(2.40) 
$$Z(x) = (D(\nabla)F(x)^{\top})^{\top}P + \widetilde{Z}(x),$$

there appears the matrix P of size  $6 \times 6$  composed of the coefficient columns  $P_{(1)}, \ldots, P_{(6)}$  in (2.37). As in [34, 44] and others, we call P the polarization matrix for the elastic inclusion  $\Omega^{\bullet}$ .

By Lemma 2.6 and formula (2.36) we obtain the integral representation

$$P = -\int_{\Omega^{\bullet}} \left( D(x)^{\top} + Z^{\bullet}(x) \right)^{\top} D(\nabla)^{\top} A^{\bullet}(x) dx$$

$$(2.41) \qquad -\int_{\Omega} \left( D(x)^{\top} + Z(x) \right)^{\top} D(\nabla)^{\top} A(x) dx$$

$$-\int_{\Gamma} \left( D(x)^{\top} + Z(x) \right)^{\top} D(n(x))^{\top} \left( A^{\bullet}(x) - A(x) \right) ds_x$$

<sup>&</sup>lt;sup>2</sup>Note, that the rows of D(x) are solutions to the transmission problem which grow at infinity while  $\{Z_{(k)}, Z_{(k)}^{\bullet}\}$  decays at infinity.

Let us transform the right-hand side of (2.41). Using  $D(\nabla)^{\top}D(x) = \mathbb{I}_6$  and integrating by parts, we find

$$\begin{split} &\int_{\Omega^{\bullet}} \left( A^{\bullet}(x) - A^{0} \right) dx + \int_{\Omega} A^{e}(x) dx \\ &= \int_{\Omega^{\bullet}} \left( D(\nabla) D(x)^{\top} \right) \left( A^{\bullet}(x) - A^{0} \right) dx + \int_{\Omega} \left( D(\nabla) D(x)^{\top} \right) A^{e}(x) dx \\ &= -\int_{\Omega^{\bullet}} D(x)^{\top} D(\nabla)^{\top} \left( A^{\bullet}(x) - A^{0} \right) dx - \int_{\Gamma} D(x)^{\top} D(n(x))^{\top} \left( A^{\bullet} - A^{0} \right) ds_{x} \\ &- \int_{\Omega} D(x)^{\top} D(\nabla)^{\top} A^{e}(x) dx + \int_{\Gamma} D(x)^{\top} D(n(x))^{\top} A^{e}(x) ds_{x} \\ &= -\int_{\Omega^{\bullet}} D(x)^{\top} D(\nabla)^{\top} A^{\bullet}(x) dx - \int_{\Omega} D(x)^{\top} D(\nabla)^{\top} A(x) dx \\ &- \int_{\Gamma} D(x)^{\top} D(n)^{\top} (A^{\bullet}(x) - A(x)) ds_{x}, \end{split}$$

the last equality holds true due to  $D(\nabla)^{\top}A^0 = 0$ . Since the columns of  $\{Z, Z^{\bullet}\}$  are contained in  $\mathcal{H}$  and fulfill definition 2.2 with data given in (2.36) we may use identity (2.19) with  $\{u, u^{\bullet}\} = \{Z, Z^{\bullet}\} = v$  and obtain further

$$-\int_{\Omega^{\bullet}} Z^{\bullet\top} D(\nabla)^{\top} A^{\bullet} dx - \int_{\Omega} Z^{\top} D(\nabla)^{\top} A dx - \int_{\Gamma} Z^{\top} D(n)^{\top} \left(A - A^{\bullet}\right) ds_x$$
$$= -\int_{\Omega^{\bullet}} \left(D(\nabla) Z^{\bullet}\right)^{\top} A^{\bullet} D(\nabla) Z^{\bullet} dx - \int_{\Omega} \left(D(\nabla) Z\right)^{\top} A D(\nabla) Z dx.$$

Thus, we have another integral representation of the polarization matrix

(2.42) 
$$P = -\int_{\Omega^{\bullet}} \left( A^{0} - A^{\bullet}(x) \right) dx + \int_{\Omega} A^{e}(x) dx \\ -\int_{\Omega} \left( D(\nabla)Z \right)^{\top} A D(\nabla) Z \, dx - \int_{\Omega^{\bullet}} \left( D(\nabla)Z^{\bullet} \right)^{\top} A^{\bullet} D(\nabla) Z^{\bullet} \, dx.$$

The last two matrices are but Gram's matrices for the sets of vector functions  $\{Z_{(k)}\}$  and  $\{Z_{(k)}^{\bullet}\}$ , hence in particular, they are symmetric and non-negative. Thus we can formulate two intrinsic properties of the polarization matrix.

**Theorem 2.7.** The polarization matrix P is always symmetric. If  $A^e = 0$ , i.e.  $A(x) = A^0$  everywhere in  $\Omega$ , and  $A^{\bullet}(x) < A^0$  for  $x \in \Omega^{\bullet}$  then P is negative definite.

2.4. A homogeneous inclusion. In this section we assume that the inclusion  $\Omega^{\bullet}$  as well as the elastic space are homogeneous, i.e.,  $A^{\bullet}$ , A are constant matrices. We put

(2.43) 
$$Z^{\bullet}(x) = Z^{*}(x) - Z^{0}(x), \qquad Z^{0}(x) = D(x)^{\top} (A^{\bullet})^{-1} (A - A^{\bullet}).$$

Then the columns of  $\{Z, Z^*\}$  satisfy problem (2.6)-(2.8) with

$$f = 0, \quad f^{\bullet} = 0, \quad g^1 = 0, \quad g^0(x) = -Z^0_{(k)}(x).$$

Applying Lemma 2.6 to this problem, we derive

$$\begin{split} -P &= \int_{\Gamma} \left( D(n)^{\top} A D(\nabla) \zeta \right)^{\top} Z^{0} \, ds_{x} \\ &= -\int_{\Gamma} \left( D(n)^{\top} A D(\nabla) (D^{\top} + Z) \right)^{\top} Z \, ds_{x} + \int_{\Gamma} \left( D(n)^{\top} A^{\bullet} D(\nabla) (D^{\top} + Z^{*} + Z^{0}) \right)^{\top} Z^{*} ds_{x} \\ &= -\int_{\Gamma} \left( D(n)^{\top} A D(\nabla) Z \right)^{\top} Z \, ds_{x} + \int_{\Gamma} \left( D(n)^{\top} A^{\bullet} D(\nabla) Z^{*} \right)^{\top} Z^{*} ds_{x} \\ &- \int_{\Gamma} \left( (\underline{2} A D (n)^{\top} A )^{\top} Z \, ds_{x} + \int_{\Gamma} \left( D(n)^{\top} A^{\bullet} (\mathbb{I}_{6} + (A^{\bullet})^{-1} (A - A^{\bullet})) \right) \right)^{\top} Z^{*} \, ds_{x}. \end{split}$$

The sum of the first two integrals in the right-hand side of (2.44) is equal to

(2.45) 
$$-\int_{\Omega} \left( D(\nabla)Z \right)^{\top} A D(\nabla)Z \, dx - \int_{\Omega^{\bullet}} \left( D(\nabla)Z^* \right)^{\top} A^{\bullet} D(\nabla)Z^* \, dx$$

and gives rise to a non-positive symmetric  $6 \times 6$ -matrix. The sum of the last two integrals in (2.44) coincides with

(2.46) 
$$\int_{\Gamma} \left( D(n(x))^{\top} A \right)^{\top} Z^{0}(x) \, ds_{x} = \int_{\Omega^{\bullet}} A D(\nabla) D(x)^{\top} (A^{\bullet})^{-1} (A - A^{\bullet}) \, dx$$
$$= A \left( A^{\bullet} \right)^{-1} \left( A - A^{\bullet} \right) \left| \Omega^{\bullet} \right| = A \left[ (A^{\bullet})^{-1} - A^{-1} \right] A \left| \Omega^{\bullet} \right|,$$

where  $|\Omega^{\bullet}|$  denotes the volume of the domain  $\Omega^{\bullet}$ . Thus we have proved the following assertion.

**Theorem 2.8.** If the matrix  $A^{\bullet}$  is constant and  $(A^{\bullet})^{-1} < A^{-1}$ , then the polarization matrix P is positive definite.

Certain positivity/negativity properties of the polarization matrix P can be expressed in terms of the eigenvalues  $\lambda_1, \ldots, \lambda_6$  of the matrix  $A^{-1/2}A^{\bullet}A^{-1/2}$ . This matrix is symmetric and positive definite, and hence  $\lambda_j > 0$  and the eigenvectors  $\mathbf{a}^{j} \in \mathbb{R}^{6}$  can be normalized by the condition  $(\mathbf{a}^{k})^{\top} \mathbf{a}^{j} = \delta_{j,k}, j, k = 1, \dots, 6$ . Then the columns  $\mathbf{b}^j = A^{-1/2} \mathbf{a}^j$  satisfy the formulae

(2.47) 
$$A^{\bullet}\mathbf{b}^{j} = \lambda_{j}A\mathbf{b}^{j}, \qquad \left(\mathbf{b}^{k}\right)^{\top}A\mathbf{b}^{j} = \delta_{k,j}$$

Forem 2.9. 1) If  $\lambda_j > 1$  then  $(\mathbf{b}^j)^\top P \mathbf{b}^j > 0$ . 2) If  $\lambda_j < 1$  then  $(\mathbf{b}^j)^\top P \mathbf{b}^j < 0$ . Theorem 2.9.

- 3) If  $\lambda_i = 1$  then  $(\mathbf{b}^j)^\top P \mathbf{b}^j = 0$ .

**Proof.** 1) Recalling (2.44) – (2.46), we see that  $-P \leq (A(A^{\bullet})^{-1}A - A) |\Omega^{\bullet}|$ . Thus, in virtue of (2.47),

$$-(\mathbf{b}^{j})^{\top} P \mathbf{b}^{j} \leq (\mathbf{b}^{j})^{\top} (A(A^{\bullet})^{-1}A - A) \mathbf{b}^{j}$$

$$(2.48) = (\mathbf{b}^{j})^{\top} A(\lambda_{j}^{-1} - 1) \mathbf{b}^{j} |\Omega^{\bullet}| = (\lambda_{j}^{-1} - 1) |\Omega^{\bullet}| < 0.$$

$$2) \text{ By } (2.42) \text{ we have } P \leq (A^{\bullet} - A) |\Omega^{\bullet}| \text{ and }$$

(2.42), we have 
$$T \leq (A^{\bullet} - A)|M^{\bullet}|$$
 and  
(2.49)  
 $(\mathbf{b}^{j})^{\top}P\mathbf{b}^{j} \leq (\mathbf{b}^{j})^{\top}(A^{\bullet} - A)\mathbf{b}^{j}|\Omega^{\bullet}| = (\mathbf{b}^{j})^{\top}A(\lambda_{j} - 1)\mathbf{b}^{j}|\Omega^{\bullet}| = (\lambda_{j} - 1)|\Omega^{\bullet}| < 0$ 

3) Repeating calculations (2.48) and (2.49), we change "< 0" for "= 0" to see the assertion.  $\hfill \Box$ 

2.5. Affine transformations. Again we consider the case of homogeneous solids, i.e. A and  $A^{\bullet}$  are constant matrices. In addition, we assume that the inclusion  $\Omega_h^{\bullet}$  is defined through rescaling:

(2.50) 
$$\Omega_h^{\bullet} = \{x : h^{-1}x \in \Omega^{\bullet}\},\$$

where h > 0 is the similarity coefficient (cf. Remark 1.3). Since the matrix function D(x) depends linearly on the variables  $x_j$ , the solution  $\zeta^h$  of the homogeneous elasticity problem for the composite elastic space  $\Omega_h \cup \Omega_h^{\bullet}$  is related to the solution  $\zeta$  by the formula

$$\zeta^h(x) = h^{-1}\zeta(hx)$$

Thus, in view of formula (2.40), we obtain that

$$P(\Omega_h^{\bullet}) = h^{-3} P(\Omega^{\bullet}) \; .$$

In [17, 18] the affine transformation

$$(2.52) x \mapsto \hat{x} = tx$$

is applied to the elasticity problem in three spatial dimensions and the notion of algebraically equivalent anisotropic media (see [1, 14]) is used to evaluate the fundamental matrix solution  $\hat{F}(\hat{x}) = (t^{\top})^{-1}F(t^{-1}\hat{x})t^{-1}$ . Thereby,  $t = (t_{jk})_{j,k=1}^3$ is an arbitrary, not necessarily orthogonal, matrix of size  $3 \times 3$ . In view of the coordinate dilatation (2.50) we may assume that

$$(2.53) det(t) = 1$$

i.e., the affine transformation preserves volume. As verified in [17, 18] matrices  $A, A^{\bullet}$  are transformed in the composite plane  $\widehat{\Omega} \cup \widehat{\Omega}^{\bullet} = t\Omega \cup t\Omega^{\bullet}$  into the new Hooke's matrices

(2.54) 
$$\widehat{A} = TAT^{\top} , \quad \widehat{A}^{\bullet} = TA^{\bullet}T^{\top}$$

where the  $(6 \times 6)$ -matrix T depends on the entries of t in the following way

$$T = \begin{pmatrix} t_{11}^2 & t_{12}^2 & t_{13}^2 & \sqrt{2} t_{12} t_{13} & \sqrt{2} t_{11} t_{13} & \sqrt{2} t_{11} t_{12} \\ t_{21}^2 & t_{22}^2 & t_{23}^2 & \sqrt{2} t_{22} t_{23} & \sqrt{2} t_{21} t_{23} & \sqrt{2} t_{21} t_{22} \\ t_{31}^2 & t_{32}^2 & t_{33}^2 & \sqrt{2} t_{32} t_{33} & \sqrt{2} t_{31} t_{33} & \sqrt{2} t_{31} t_{32} \\ \sqrt{2} t_{21} t_{31} & \sqrt{2} t_{22} t_{32} & \sqrt{2} t_{23} t_{33} & t_{23} t_{32} + t_{22} t_{33} & t_{23} t_{31} + t_{21} t_{33} & t_{22} t_{31} + t_{21} t_{32} \\ \sqrt{2} t_{11} t_{31} & \sqrt{2} t_{12} t_{22} & \sqrt{2} t_{13} t_{33} & t_{13} t_{32} + t_{12} t_{33} & t_{13} t_{31} + t_{11} t_{33} & t_{12} t_{31} + t_{11} t_{32} \\ \sqrt{2} t_{11} t_{21} & \sqrt{2} t_{12} t_{22} & \sqrt{2} t_{13} t_{23} & t_{13} t_{22} + t_{12} t_{23} & t_{13} t_{21} + t_{11} t_{23} & t_{12} t_{21} + t_{11} t_{22} \end{pmatrix}$$

From the calculations in [18] it follows that the polarization matrix  $\widehat{P}(\widehat{\Omega}^{\bullet})$  for the algebraically equivalent composite plane  $\widehat{\Omega} \cup \widehat{\Omega}^{\bullet}$  takes the form

(2.55) 
$$\widehat{P}(\widehat{\Omega}^{\bullet}) = TP(\Omega^{\bullet})T^{\top} .$$

Formula (2.55) becomes explicit if the original matrix  $P(\Omega^{\bullet})$  is known. If  $\overline{\Omega}^{\bullet}$  is a cavity, then affin transformations of type (2.52) are useful to simplify the anisotropic properties of the medium. For example, in two spatial dimensions it is known that any anisotropic material is algebraically equivalent to an orthotropic material with four symmetry axes (see [1, 14]).

2.6. An application of the Eshelby theorem. Again we assume that the Hooke matrices A and  $A^{\bullet}$  are constant, and the inclusion  $\Omega^{\bullet}$  is an ellipsoid given by the relation

$$(2.56)$$
  $|tx| < t_0$ 

where  $t_0 > 0$  is a real number and  $t \in \mathbb{R}^{3\times 3}$  a fixed  $3 \times 3$  matrix with det t = 1. It is known since the work of Eshelby [11] (see [16, 29] and [13, 15], where the three-dimensional case is considered as well) that a constant deformation  $\varepsilon^{\infty}$  at infinity generates constant strains and stresses in the ellipsoidal inclusion  $\Omega^{\bullet}$ . In our notation this means that the formal matrix solution (2.38) of the homogeneous problem (2.6), (2.7) satisfies

$$(2.57) D(\nabla)\zeta^{\bullet} = Q, x \in \Omega^{\bullet}$$

where Q is a real  $6 \times 6$  matrix. We call Q the Eshelby-Matrix, it depends on the Hooke-matrices A,  $A^{\bullet}$ , and the position and size of the ellipsoidal inclusion (2.56).

To find the relation between the polarization matrix  $P = P(\Omega^{\bullet})$  and the Eshelby matrix Q, we recall that the vector functions (2.37) satisfy problem (2.6)–(2.8) with the right-hand sides (2.36). Since A,  $A^{\bullet}$  are constant we have  $f_{(k)}^{\bullet} = f_{(k)} = 0$ in addition. The matrix  $\{Z, Z^{\bullet}\}$  admits the asymptotic form (2.40) and can be regarded as a solution in  $\mathcal{H}$  to the elasticity problem in the *whole space* (recall the notation  $\mathcal{L} = D(-\nabla)^{\top} A D(\nabla)$ )

(2.58) 
$$D(-\nabla)^{\top}AD(\nabla)Z(x) = 0, \qquad x \in \Omega$$
$$D(-\nabla)^{\top}AD(\nabla)Z^{\bullet}(x) = F^{\bullet} := D(-\nabla)^{\top}(A - A^{\bullet})D(\nabla)Z^{\bullet}, \quad x \in \Omega^{\bullet}$$

with a jump in the Neumann data on the surface  $\Gamma$ 

(2.59) 
$$D(n(x))^{\top}AD(\nabla)Z(x) - D(n(x))^{\top}AD(\nabla)Z^{\bullet}(x) = G^{1}(x) := D(n(x))^{\top}(A^{\bullet} - A)(\mathbb{I}_{6} + D(\nabla)Z^{\bullet}(x)).$$

Evidently,  $\zeta(x) = D(x)^{\top}$  if  $a = A^{\bullet}$  in (2.36). Comparing (2.40) and (2.29), Lemma 2.6 leads to the representation

$$-P = \int_{\Omega^{\bullet}} F^{\bullet} dx + \int_{\Gamma} G^{1}(x) ds_{x} =$$
  
= 
$$\int_{\Omega^{\bullet}} D(x) D(\nabla)^{\top} (A^{\bullet} - A) D(\nabla) Z^{\bullet}(x) dx +$$
  
+ 
$$\int_{\Gamma} D(x) D(n(x))^{\top} (A^{\bullet} - A) (\mathbb{I}_{6} + D(\nabla) Z^{\bullet}(x)) ds_{x}$$
  
= 
$$\int_{\Omega^{\bullet}} (A - A^{\bullet}) (\mathbb{I}_{6} + D(\nabla) Z^{\bullet}(x)) ds_{x}.$$

Finally, the definition (2.57) of the Eshelby matrix Q yields the desired relation

(2.60) 
$$P = (A^{\bullet} - A)(\mathbb{I}_6 + Q)mes_3\Omega^{\bullet}.$$

Special properties of the polarization matrix P as outlined in Section 2.3 lead to some properties of the Eshelby matrix which are not known yet. Namely, by Theorem 2.7, we derive

**Corollary 2.10.** Let Q be the Eshelby matrix defined in (2.57), then

(2.61) 
$$(A^{\bullet} - A)Q = Q^{\top}(A^{\bullet} - A)$$

(2.62) 
$$(A^{\bullet} - A)Q = \frac{1}{|\Omega^{\bullet}|} \Big( \int_{\Omega} (D(\nabla)Z(x)^{\top}AD(\nabla)Z(x)dx + \int_{\Omega^{\bullet}} (D(\nabla)Z^{\bullet}(x)^{\top}A^{\bullet}D(\nabla)Z^{\bullet}(x)dx \Big)$$

We introduce the symmetrized Eshelby matrix

$$\mathcal{Q} = \frac{1}{2}((A^{\bullet} - A)Q + Q^{\top}(A^{\bullet} - A)),$$

which is symmetric and positive due to Corollary 2.10. Then the formula (2.60) turns into

$$P = (A^{\bullet} - A + \mathcal{Q})mes_3\Omega^{\bullet}.$$

### 3. Shape sensitivity analysis for polarization matrices

Direct approach of the shape sensitivity analysis is used in two spatial dimensions. There is no major difficulty to apply the same approach in the three spatial dimensions, however we prefer to perform such an analysis in the framework of standard boundary variation technique with the material derivatives and the shape gradients of energy functionals. In this way we show that two general approaches of the shape sensitivity analysis are applicable for polarization matrices.

3.1. Two dimensional problems. We start with the same assumptions as in Section 2.4, only as a two-dimensional problem, i.e.  $\mathbb{R}^2 = \Omega \cup \Omega^{\bullet}$ , where  $\Omega^{\bullet} \subset \mathbb{R}^2$  is bounded by a smooth contour  $\Gamma$ , and the elastic materials which fill up  $\Omega^{\bullet}$  and  $\Omega = \mathbb{R}^2 \setminus \Omega^{\bullet}$  are homogeneous with constant Hooke's matrices of size  $3 \times 3$  (see Section 1.4).

In a neighborhood  $\mathcal{U}$  of  $\Gamma$  we introduce a curvilinear coordinate system (s, n), where n is the oriented distance to  $\Gamma$ , n > 0 in  $\Omega^{\bullet}$ , and s is the arc length on  $\Gamma$ . In our notation a point on  $\Gamma$  is identified with its coordinate s. Moreover, a function  $x \mapsto v(x)$ , after the change of variables is still denoted v(n, s). By an appropriate rescaling, the diameter of the inclusion becomes 1, so that all coordinates are dimensionless. Given a small parameter h and a function  $H \in C^2(\Gamma)$ , we introduce the perturbed contour

(3.1) 
$$\Gamma_h = \{ x \in \mathcal{U} : s \in \Gamma , \quad n = hH(s) \}$$

it becomes the boundary of the perturbed inclusion  $\Omega_h^{\bullet}$ , while  $\Omega_h = \mathbb{R}^2 \setminus \Omega_h^{\bullet}$ . We use the notation introduced in Sections 2.1 and 1.4. The polarization matrix P(h) of size  $3 \times 3$  for the inclusion  $\Omega_h^{\bullet}$  is determined from the transmission boundary value problem

(3.2) 
$$D(-\nabla)^{\top}AD(\nabla)Z_{(k)}^{h}(x) = 0, \qquad x \in \Omega_{h}$$

(3.3) 
$$D(-\nabla)^{\top} A^{\bullet} D(\nabla) Z_{(k)}^{h \bullet}(x) = 0, \qquad x \in \Omega_h^{\bullet}$$

(3.4) 
$$D(n^{n}(x))^{\top} (AD(\nabla)Z^{n}_{(k)}(x) - A^{\bullet}D(\nabla)Z^{n\bullet}_{(k)}(x))$$
$$= -D(n^{h}(x))^{\top}(A - A^{\bullet})\mathbf{e}_{k},$$
$$x \in \Gamma_{h},$$

(3.5) 
$$Z^h_{(k)}(x) = Z^{h\bullet}_{(k)}(x) , \qquad x \in \Gamma_h$$

where  $\mathbf{e}_k = (\delta_{1,k}, \delta_{2,k}, \delta_{3,k})$ . The solutions  $Z_{(k)}^h, Z_{(k)}^{h\bullet}$  exist and  $(2 \times 3)$ -matrix  $Z^h = (Z^{h1}, Z^{h2}, Z^{h3})$  admits the asymptotic form

(3.6) 
$$Z^{h}(x) = (D(\nabla)F(x)^{\top})^{\top}P(h) + O(|x|^{-2})$$

(cf. (1.24)). We are going to find the second term in the asymptotics of the polarization matrix

$$(3.7) P(h) = P + h\mathcal{P} + \dots$$

It is reasonable to suppose that the solutions  $\{Z^k, Z^{\bullet k}\}$  and the matrix P are known for the unperturbed inclusion  $\Omega^{\bullet} = \Omega_0^{\bullet}$ . Then, we need to find the correction terms in the expansions

(3.8) 
$$Z^{h}_{(k)}(x) = Z^{k}(x) + \mathcal{Z}^{k}(x) + \dots$$
$$Z^{h}_{(k)}(x) = Z^{\bullet k}(x) + \mathcal{Z}^{\bullet k}(x) + \dots$$

According to (2.38) the matrix functions  $\zeta^h = D^\top + Z^h$  and  $\zeta = D^\top + Z$  solve the homogeneous problem (3.2)-(3.5) in  $\Omega_h \cup \Omega_h^{\bullet}$  and  $\Omega \cup \Omega^{\bullet}$ , respectively. That is why, it is more convenient to consider the expansions of theirs columns

(3.9) 
$$\zeta_{(k)}^{h}(x) = \zeta^{k}(x) + \mathcal{Z}^{k}(x) + \dots,$$
$$\zeta_{(k)}^{h\bullet}(x) = \zeta^{\bullet k}(x) + \mathcal{Z}^{\bullet k}(x) + \dots,$$

which immediately follow from (3.8).

Since the boundary  $\Gamma$  is smooth, the vector functions  $\zeta^k$  and  $\zeta^{\bullet k}$  can be extended in the Sobolev class  $H^2$  from  $\Omega$  and  $\Omega^{\bullet}$  onto  $\Omega \cup \mathcal{U}$  and  $\Omega^{\bullet} \cup \mathcal{U}$ , respectively. The extensions are still denoted by  $\zeta^k$  and  $\zeta^{\bullet k}$ . Clearly,  $\mathcal{Z}^k$  and  $\mathcal{Z}^{\bullet k}$  have to verify the homogeneous elasticity system

(3.10) 
$$D(-\nabla)^{\top} A D(\nabla) \mathcal{Z}^{k}(x) = 0 , \quad x \in \Omega ,$$

$$(3.11) D(-\nabla)^{\top} A^{\bullet} D(\nabla) \mathcal{Z}^{\bullet k}(x) = 0 , \quad x \in \Omega^{\bullet} .$$

It remains to evaluate the main parts of discrepancies in the homogeneous transmission conditions (3.4) and (3.5) which appear due to shift (3.1) of the contact contour.

We introduce the projections  $\zeta_n$  and  $\zeta_s$  of the displacement vector  $\zeta = (\zeta_1, \zeta_2)$ on the axes *n* and *s*, respectively,

(3.12) 
$$\begin{aligned} \zeta_n(n,s) &= n_1(s)\zeta_1(n,s) + n_2(s)\zeta_2(n,s) ,\\ \zeta_s(n,s) &= -n_2(s)\zeta_1(n,s) + n_1(s)\zeta_2(n,s) ,\end{aligned}$$

where  $\mathbf{n} = (n_1, n_2)^{\top}$  stands for the unit normal vector on  $\Gamma$  interior to the inclusion  $\Omega^{\bullet}$ . The curvilinear components of the strain tensor  $\boldsymbol{\varepsilon}(\zeta)$  take the form

(3.13) 
$$\begin{aligned} \varepsilon_{nn}(\zeta) &= n_1^2 \varepsilon_{11}(\zeta) + n_2^2 \varepsilon_{22}(\zeta) + 2n_1 n_2 \varepsilon_{12}(\zeta) ,\\ \varepsilon_{ss}(\zeta) &= n_2^2 \varepsilon_{11}(\zeta) + n_1^2 \varepsilon_{22}(\zeta) - 2n_1 n_2 \varepsilon_{12}(\zeta) ,\\ \varepsilon_{ns}(\zeta) &= \varepsilon_{sn}(\zeta) = n_1 n_2 (\varepsilon_{11}(\zeta) - \varepsilon_{22}(\zeta)) + (n_1^2 - n_2^2) \varepsilon_{12}(\zeta) .\end{aligned}$$

In terms of displacements the components of the strain tensor are expressed as follows:

(3.14) 
$$\varepsilon_{nn}(\zeta) = \partial_n \zeta_n , \quad \varepsilon_{ss}(\zeta) = J^{-1}(\partial_s \zeta_s + \varkappa \zeta_n) ,$$
$$\varepsilon_{ns}(\zeta) = \varepsilon_{sn}(\zeta) = \frac{1}{2}(\partial_n \zeta_s + J^{-1}(\partial_s \zeta_n - \varkappa \zeta_s)) ,$$

where  $\partial_n = \partial/\partial n$ ,  $\partial_s = \partial/\partial s$ ,  $J(n,s) = 1 + n\varkappa(s)$  is the Jacobian and  $\varkappa(s)$  is the curvature of the arc  $\Gamma$  at the point s.

The Hooke's law (1.19) in the coordinates (n, s) takes the form

$$\begin{pmatrix} \sigma_{nn}(\zeta;n,s) \\ \sigma_{ss}(\zeta;n,s) \\ \sqrt{2}\sigma_{ns}(\zeta;n,s) \end{pmatrix} = \mathcal{A}(s) \begin{pmatrix} \varepsilon_{nn}(\zeta;n,s) \\ \varepsilon_{ss}(\zeta;n,s) \\ \sqrt{2}\varepsilon_{ns}(\zeta;n,s) \end{pmatrix} , \quad \mathcal{A}(s) = \Theta(s)^{\top} \mathcal{A}\Theta(s) ,$$

where the matrix  $\Theta(s)$  is given by formula (1.18) with  $\cos \vartheta = n_1$  and  $\sin \vartheta = n_2$ . For the transmission condition (3.5) the Taylor formula

(3.16) 
$$\zeta(hH(s), s) = \zeta(0, s) + hH(s)\partial_n\zeta(0, s) + O(h^2)$$

readily yields

(3.17) 
$$\mathcal{Z}^{k}(0,s) - \mathcal{Z}^{\bullet k}(0,s) = H(s)(\partial_{n}\zeta^{k}(0,s) - \partial_{n}\zeta^{\bullet k}(0,s)) , \quad s \in \Gamma .$$

Since  $(\partial_n, J(n, s)^{-1}\partial_s)$  is the gradient operator in the curvilinear coordinates, the unit normal  $n^h$  and the tangential vector  $s^h$  on  $\Gamma_h$  have the components

$$n_n^h(s) = s_s^h(s) = j^h(s)^{-1/2}, \quad n_s^h(s) = -s_n^h(s) = -hj^h(s)^{-1/2}\partial_s H(s),$$

where  $j^{h}(s)$  stands for the normalizing factor  $1 + h^{2}H'(s)^{2}$  and  $H' = \partial_{s}H$ . Hence

(3.18)  

$$\begin{aligned} \sigma_{n^{h}n^{h}}(\zeta + h\mathcal{Z}; hH(s), s) &= \sigma_{nn}(\zeta; 0, s) + h(H(s)\partial_{n}\sigma_{nn}(\zeta; 0, s) \\ &-2H'(s)\sigma_{ns}(\zeta; 0, s) + \sigma_{nn}(\mathcal{Z}; 0, s)) + O(h^{2}) , \\ \sigma_{n^{h}s^{h}}(\zeta + h\mathcal{Z}; hH(s), s) &= \sigma_{ns}(\zeta; 0, s) + h(H(s)\partial_{n}\sigma_{ns}(\zeta; 0, s) \\ &+H'(s)(\sigma_{nn}(\zeta; 0, s) - \sigma_{ss}(\zeta; 0, s)) + \sigma_{ns}(\mathcal{Z}; 0, s)) + O(h^{2}) .
\end{aligned}$$

On the other hand, the equilibrium equations in the coordinates (n, s) take the form

$$\begin{aligned} -\partial_n \sigma_{nn}(\zeta) - J^{-1}(\partial_s \sigma_{ns}(\zeta) + \varkappa(\sigma_{nn}(\zeta) - \sigma_{ss}(\zeta))) &= 0 , \\ -\partial_n \sigma_{ns}(\zeta) - J^{-1}(\partial_s \sigma_{ss}(\zeta) + 2\varkappa\sigma_{ns}(\zeta)) &= 0 \end{aligned}$$

and for n = 0 we obtain

(3.19) 
$$\partial_n \sigma_{nn}(\zeta;0,s) = -\partial_s \sigma_{ns}(\zeta;0,s) - \varkappa(\sigma_{nn}(\zeta;0,s) - \sigma_{ss}(\zeta;0,s)) , \partial_n \sigma_{ns}(\zeta;0,s) = -\partial_s \sigma_{ss}(\zeta;0,s) - 2\varkappa\sigma_{ns}(\zeta;0,s)) .$$

Now, we are able to conclude on the second transmission condition for  $\mathbb{Z}^k, \mathbb{Z}^{\bullet k}$ . Since  $\zeta^k, \zeta^{\bullet k}$  satisfy the homogeneous transmission conditions on the unperturbed contour  $\Gamma$ , the following identities are still valid on  $\Gamma$ 

(3.20) 
$$\zeta_n^k = \zeta_n^{\bullet k}$$
,  $\zeta_s^k = \zeta_s^{\bullet k}$ ,  $\sigma_{nn}(\zeta^k) = \sigma_{nn}(\zeta^{\bullet k})$ ,  $\sigma_{ns}(\zeta^k) = \sigma_{ns}(\zeta^{\bullet k})$ ,

this considerably simplifies the above formulae. In particular, taking into account the second relations in (3.18), (3.19) we have

$$\begin{split} \sigma_{ns}(\mathcal{Z}^{k}) &- \sigma_{ns}^{\bullet}(\mathcal{Z}^{\bullet k}) = -H\left(\partial_{n}\sigma_{ns}(\zeta^{k}) - \partial_{n}\sigma_{ns}^{\bullet}(\zeta^{\bullet k})\right) - H'\left(\{\sigma_{nn}(\zeta^{k}) - \sigma_{nn}^{\bullet}(\zeta^{\bullet k})\}\right) \\ &+ H'\left(\sigma_{ss}(\zeta^{k}) - \sigma_{ss}^{\bullet}(\zeta^{\bullet k})\right) = H\left(\partial_{s}\sigma_{ss}(\zeta^{k}) - \partial_{s}\sigma_{ss}^{\bullet}(\zeta^{\bullet k}) + 2\varkappa\{(\sigma_{ns}(\zeta^{k}) - \sigma_{ns}^{\bullet}(\zeta^{\bullet k})\})\right) \\ &+ H'\left(\sigma_{ss}(\zeta^{k}) - \sigma_{ss}^{\bullet}(\zeta^{\bullet k})\right) = \partial_{s}H\left(\sigma_{ss}(\zeta^{k}) - \sigma_{ss}^{\bullet}(\zeta^{\bullet k})\right) \ , \end{split}$$

note that the terms in  $\{\}$  vanish due to (3.20). Similar calculations, in view of the first relations in (3.18), (3.19) lead to the couple of transmition conditions

$$(3.21) \quad \sigma_{nn}(\mathcal{Z}^{k}; 0, s) - \sigma_{nn}(\mathcal{Z}^{\bullet k}; 0, s) = -\varkappa(s)H(s)(\sigma_{ss}(\zeta^{k}; 0, s) - \sigma_{ss}(\zeta^{\bullet k}; 0, s)) , \sigma_{ns}(\mathcal{Z}^{k}; 0, s) - \sigma_{ns}(\mathcal{Z}^{\bullet k}; 0, s) = \partial_{s}(H(s)(\sigma_{ss}(\zeta^{k}; 0, s) - \sigma_{ss}(\zeta^{\bullet k}; 0, s)) , \quad s \in \Gamma .$$

Problems (3.10), (3.11), (3.17), (3.21) with k = 1, 2, 3 admit decaying matrix solutions

$$\mathcal{Z} = (\mathcal{Z}^1, \mathcal{Z}^2, \mathcal{Z}^3) , \quad \mathcal{Z}^{\bullet} = (\mathcal{Z}^{\bullet 1}, \mathcal{Z}^{\bullet 2}, \mathcal{Z}^{\bullet 3})$$

of the form

(3.22) 
$$\mathcal{Z}(x) = (D(\nabla)F(x)^{\top})^{\top}\mathcal{P} + O(|x|^{-2})$$

(cf. (3.6)). According to Lemma 2.6, the entries of  $(3 \times 3)$ -matrix  $\mathcal{P}$  in (3.22) and (3.7) have the integral representation

(3.23)  
$$\mathcal{P}_{jk} = \int_{\Gamma} (\zeta^j)^\top (\sigma^{(n)}(\mathcal{Z}^k) - \sigma^{\bullet(n)}(\mathcal{Z}^{\bullet k})) ds_x - \int_{\Gamma} (\mathcal{Z}^k - \mathcal{Z}^{\bullet k})^\top \sigma^{(n)}(\zeta^j) ds_x =: I_1 - I_2$$

Note, that in view of the homogeneous conditions (3.5) and (3.4), the identities  $\zeta^{j} = \zeta^{\bullet j}$  and  $\sigma^{(n)}(\zeta^{j}) = \sigma^{\bullet(n)}(\zeta^{\bullet j})$  hold true on  $\Gamma$ , which has been taken into account in (3.23).

Using formulae (3.14) and (3.20) it follows that

$$\partial_n \zeta^k - \partial_n \zeta^{\bullet k} = 2\varepsilon_{ns}(\zeta^k) - 2\varepsilon_{ns}(\zeta^{\bullet k}) \quad on \ \Gamma$$

and, by (3.17),

(3.24) 
$$I_2 = -\int_{\Gamma} (\varepsilon_{nn}(\zeta^k) - \varepsilon_{nn}(\zeta^{\bullet k})) \sigma_{nn}(\zeta^j) + 2(\varepsilon_{ns}(\zeta^k) - \varepsilon_{ns}(\zeta^{\bullet k})) \sigma_{ns}(\zeta^j) ds_x .$$

Furthermore, applying (3.21), (3.20), (3.14) and integrating by parts on the contour  $\Gamma$  result in

$$(3.25)$$

$$I_{1} = \int_{\Gamma} (\zeta_{s}^{j} \partial_{s} (H(\sigma_{ss}(\zeta^{k}) - \sigma_{ss}^{\bullet}(\zeta^{\bullet k}))) - \zeta_{n}^{j} \varkappa H(\sigma_{ss}(\zeta^{k}) - \sigma_{ss}^{\bullet}(\zeta^{\bullet k}))) ds_{x}$$

$$- \int_{\Gamma} H(\sigma_{ss}(\zeta^{k}) - \sigma_{ss}^{\bullet}(\zeta^{\bullet k})) (\partial_{s}\zeta_{s}^{j} + \varkappa \zeta_{n}^{j}) ds_{x} - \int_{\Gamma} H(\sigma_{ss}(\zeta^{k}) - \sigma_{ss}^{\bullet}(\zeta^{\bullet k})) \varepsilon_{ss}(\zeta^{j}) ds_{x} .$$

In order to explain the physical sense of the obtained expression, we recall the notion of the surface enthalpy [48, 38], which is common in many applications in mechanics, namely, the integral

(3.26) 
$$\Xi(\zeta) = \frac{1}{2} \int_{\Gamma} \xi(\zeta, \zeta) ds_x$$

with the density<sup>3</sup>

$$\xi(\zeta,\eta) = \sigma_{nn}(\zeta)\varepsilon_{nn}(\eta) + \sigma_{ns}(\zeta)\varepsilon_{ns}(\eta) + \sigma_{sn}(\zeta)\varepsilon_{sn}(\eta) - \varepsilon_{ss}(\zeta)\sigma_{ss}(\eta) + \sigma_{sn}(\zeta)\varepsilon_{sn}(\eta) + \sigma_{sn}(\zeta)\varepsilon_{sn}(\eta)$$

 $<sup>^{3}</sup>$ The quadratic functional (3.26) is but a Gibbs functional, obtained from the surface energy functional by the partial Lagrange transformation for the tangential components of the stress/strain state [].

We emphasize, that all terms evaluated for  $\zeta$  and  $\zeta^{\bullet}$  are continuous on  $\Gamma$  in view of the homogeneous transmission conditions (3.5), (3.4), while all terms evaluated for  $\eta$  may have jumps over  $\Gamma$ .

From (3.23) - (3.25) it is straightforward to obtain

(3.27) 
$$\mathcal{P}_{jk} = \int_{\Gamma} H(s)\xi(\zeta^j, \zeta^k; s)ds_x - \int_{\Gamma} H(s)\xi^{\bullet}(\zeta^{\bullet j}, \zeta^{\bullet k}; s)ds_x \ .$$

In other words, the matrix  $\mathcal{P}$  in (3.7) is given by the jumps of the weighted enthalpy obtained for the special solutions  $\zeta$  of the homogeneous problem (3.2)- (3.5) for the composite plane  $\Omega \cup \Omega^{\bullet}$  with the original contact contour  $\Gamma$ .

We have performed the formal asymptotic analysis which can be justified in the same way as in [48] for elasticity problems in domains with rapidly oscillating boundaries (but with the serious simplifications, see also [37] for a phase transition problem in the same framework).

**Proposition 3.1.** The polarization matrix P(h) of the composite plane  $\Omega_h \cup \Omega_h^{\bullet}$  with the perturbed contact contour (3.1) has the asymptotic form (3.7) where the entries of matrix  $\mathcal{P}$  are provided in (3.27), and the remainder is of order  $O(h^2)$ .

Let us consider the elastic plane with the hole  $\Omega_h^{\bullet}$  bounded by the perturbed contour (3.1) (cf. Section 1.2). The formula (3.7) in Proposition 3.1 crucially simplifies

(3.28)  
$$\mathcal{P}_{jk} = -\int_{\Gamma} H(s)\varepsilon_{ss}(\zeta^{j}; 0, s)\varepsilon_{ss}(\zeta^{k}; 0, s)ds$$
$$= -\int_{\Gamma} H(s) \left(\mathcal{A}^{-1}(s)\right)_{22}\sigma_{ss}(\zeta^{j}; 0, s)\sigma_{ss}(\zeta^{k}; 0, s)ds$$

since  $A^{\bullet} = 0$  and  $\sigma_{nn}(\zeta^p) = \sigma_{ns}(\zeta^p) = 0$  on  $\Gamma$  and, moreover, inverting the Hook's law (3.14) we obtain

$$\begin{split} \varepsilon_{ss}(\zeta^{j};0,s) &= \left(\mathcal{A}(s)^{-1}\right)_{21} \sigma_{nn}(\zeta^{p};0,s) + \\ &+ \left(\mathcal{A}(s)^{-1}\right)_{22} \sigma_{ss}(\zeta^{j};0,s) + \sqrt{2} \left(\mathcal{A}(s)^{-1}\right)_{23} \sigma_{ns}(\zeta^{j};0,s) \\ &= \left(\mathcal{A}(s)^{-1}\right)_{22} \sigma_{ss}(\zeta^{j};0,s), \quad s \in \Gamma \;. \end{split}$$

Here,  $\zeta^{j}(x) = D^{j}(x) + Z^{j}(x)$  are solutions to the homogeneous exterior elasticity problem (1.22) with linear growth in infinity. The entry  $(\mathcal{A}(s)^{-1})_{22}$  of the compliance matrix  $\mathcal{A}(s)^{-1}$  is positive, and, hence, the matrix  $\mathcal{P}$  with elements (3.28) is positive definite in the case when the hole enlarges, that is for H(s) < 0 (recall that n is the outward normal with respect to  $\Omega = \mathbb{R}^{2} \setminus \overline{\Omega^{\bullet}}$ ). In contrast, shrinking the hole leads to a decrease of eigenvalues of the polarization matrix P.

**Remark 3.2.** The virtual mass matrix m(h) for the exterior Neumann problem in  $\Omega_h$  (see Section 1.2) gets the similar expansion

(3.29) 
$$m(h) = m + h\mathcal{M} + O(h^2) ,$$
$$\mathcal{M}_{jk} = -\int_{\Gamma} H(s)\partial_s \zeta^j(0,s)\partial_s \zeta^k(0,s)ds ,$$

where m is  $(2 \times 2)$ -matrix with the entries  $m_{jk}$  in (1.3) and  $\zeta^j(x) = x_j + z^j(x)$ are given by the solutions to homogeneous problem (1.1) with the linear growth at infinity. The above conclusion on the positivity/negativity of the matrix  $\mathcal{P}$  remains valid for the matrix  $\mathcal{M}$  with elements (3.29).

3.2. Shape sensitivity analysis in three spatial dimensions. The classical shape sensitivity analysis in smooth domains can be applied in order to derive the shape derivatives of the polarization matrix. In the special case  $g^0 = 0$  in (2.7) the weak solution to the transmission problem (see Definition 2.2) minimizes the energy functional

(3.1) 
$$J_0(\Gamma) = \frac{1}{2} (AD(\nabla)u), D(\nabla)u)_{\Omega} + \frac{1}{2} (A^{\bullet}D(\nabla)u^{\bullet}, D(\nabla)u^{\bullet})_{\Omega^{\bullet}} - (f, u)_{\Omega} - (f^{\bullet}, u^{\bullet})_{\Omega^{\bullet}} - \langle g^1, u = u^{\bullet} \rangle_{\Gamma} =: \frac{1}{2} a(u, u) - L(u).$$

Recalling the representation (2.42) we observe that the entries of the polarization matrix can be obtained using such functionals which simplifies the derivation. Thus we start with an auxiliary result on material derivatives of the minimizers to (3.1). which seems to be interesting on its own. We point out that, in view of the representation (3.35) of the polarization matrix, the shape derivatives of the polarization matrix P with respect to the perturbations of the interface  $\Gamma$  can be deduced from the shape differentiability of the energy functional (3.1), the resulting shape derivatives are given by formula (3.36). The existence of the shape derivative  $dJ(\Gamma; V)$ of the functional (3.1) follows by Lemma 3.5 combined with the standard results on the differentiability of volume and surface i ntegrals [55] which are listed below, in Lemma 3.3. The result is established by the differentiability of the functional (3.31) with respect to the parameter t at t = 0. Another problem, important for numerical applications of our results, is the identification of the obtained shape gradient  $q_{\Gamma}$  given in formula (3.33). The actual form of the shape gradient can be given by the derivation with respect to t in the variable domain setting of our problem. We exploit to this end the shape differentiability of the energy type shape functionals, taking into account the decomposition of P in (3.26), (3.27) combined with the representations (3.28), (3.29) for the entries of the functionals in (3.1). All steps in this derivation of formula (3.36) can be performed along the lines of [55].

3.3. Deformations of interfaces. Let  $\Xi \subset \mathbb{R}^3$  be a domain with smooth compact boundary  $\Gamma$  of class  $C^{2,\alpha}$  at least, we can think of  $\Xi \in \{\Omega, \Omega^{\bullet}\}$ , and  $V \in C_0^k(\mathbb{R}^3)^3$ ,  $k \geq 1$ , be a fixed given mapping with compact support in an open neighbourhood of  $\Gamma$ . To V we relate the family of diffeomorphisms  $T_t : \mathbb{R}^3 \mapsto \mathbb{R}^3$  with inverse  $T_t^{-1}$ defined by

$$T_t(x) := x + tV(x) = (I + tV)(x), \quad t \in [0, \epsilon_0).$$

We denote the change of variables by

$$y(x) := T_t(x),$$

and also introduce the families of transported domains and interfaces

(3.2) 
$$\Xi_t := T_t(\Xi), \quad \Gamma_t := T_t(\Gamma).$$

If 
$$g(t, \cdot) := g_t \in H^1(\Xi_t)$$
 for  $t \in [0, \epsilon_0)$ , then  
(3.3)  $g^t := g_t \circ T_t \in H^1(\Xi)$ 

and with  $g = g(0, \cdot) \in H^1(\Xi)$  the strong (weak) material derivative is defined as

$$\dot{g}(V) = \lim_{t \to 0} \frac{1}{t} (g_t \circ T_t - g) = \lim_{t \to 0} \frac{1}{t} (g^t - g)$$

provided this limit exists strongly (weakly) in  $H^1(\Xi)$ . Thereby the Sobolev space  $H^1(\Xi)$  can be replaced by any other Sobolev space (eventually under additional regularity assumptions for V). In a similar manner, we can define  $\dot{g}$  for functions defined on  $\Gamma_t$ . If the weak material derivative exists in  $H^1(\Xi)$ , then the shape derivative  $g' \in L^2(\Xi)$  in the direction of V is defined by

$$(3.4) g' = \dot{g} - \nabla g \cdot V$$

If  $g \in H^2(\Xi)$ , then the tangential gradient  $\nabla_{\Gamma} g := \nabla_x g - (\nabla_x g \cdot n)n$  exists in  $H^{1/2}(\Gamma)$  and we can define the boundary shape derivative

(3.5) 
$$g'_{\Gamma} = \dot{g} - \nabla_{\Gamma} g \cdot V,$$

again provided  $\dot{g}$  exists in  $H^{1/2}(\Gamma)$  at least as a weak limit. In the following we deal with two kinds of functions defined in the domain  $\Xi_t$ . The first type are functions defined in the whole space  $\mathbb{R}^3$  and then restricted to  $\Xi_t$ . They appear as data for our problems, and their so-called shape and material derivatives are explicitly given [55]. The second type of functions are the solutions to boundary value problems defined in the variable domains, especially solutions to the transmission problem. For these functions the material derivatives are defined by solutions of auxiliary boundary value problems defined in the fixed domain  $\Xi$ , and there is a relation between shape and material derivatives [55]. We use the following notation for the functions and variables

(3.6)  

$$y := y(x) = T_t(x) \in \Xi_t,$$

$$\mathfrak{T}_t(x) := \nabla_x T_t(x) = (\partial y_i / \partial x_j)_{i,j=1,2,3},$$

$$\vartheta_t(x) := \det(\mathfrak{T}_t), \quad \mathfrak{T}_t^{-\top} := (\mathfrak{T}_t^{-1})^{\top}.$$

Note that  $\vartheta_t > 0$  if t is small enough. Clearly we have

(3.7) 
$$\begin{aligned} \partial_t \mathfrak{T}_t(x)|_{t=0} &= \nabla_x V(x) = \mathfrak{T}'(x), \\ \partial_t \vartheta_t(x)|_{t=0} &= \nabla_x \cdot V(x) = \vartheta'(x), \\ \partial_t \mathfrak{T}_t^{-\top}(x)|_{t=0} &= -(\nabla V(x))^{\top} = (\mathfrak{T}^{-\top})'(x), \end{aligned}$$

the last formula follows if we observe that  $\mathfrak{T}|_{t=0}$  coincides with the unit matrix  $\mathbb{I}^4$ . We recall some results on the transport of differential operators and integrals, they are used in order to obtain the derivatives with respect to the parameter t at t = 0of volume and surface integrals. For the proofs we refer to [55].

**Lemma 3.3.** For  $\Xi$ ,  $\Xi_t$ , and  $g_t$  as in (3.2) and (3.3), respectively, we have

(3.8) 
$$\int_{\Xi_t} g_t(y) dy = \int_{\Xi} g^t(x) \vartheta_t(x) dx, \quad \int_{\Gamma_t} g_t(y) ds_y = \int_{\Gamma} g^t(x) \theta_t(x) ds_x,$$

where  $\theta_t(x)$  is the surface Jacobian, i.e.  $\theta_t(x) = |\vartheta_t(x) (\mathfrak{T}_t^{-1}(x))^\top \cdot n(x)|$ , n(x) the unit normal vector in  $x \in \Gamma$ . The derivatives of the integrals (3.8) for t = 0 take

<sup>&</sup>lt;sup>4</sup>The notation  $\mathfrak{T}'(x)$  etc is consistent with (3.4), it we observe that for a sufficiently regular regular function g(t,x) defined on an open neighbourhood of  $\bigcup_{t\in[0,\epsilon_0)}\subset \mathbb{R}^4$  it follows:  $g'(x) = \partial_t g(t,x)|_{t=0}$ , and  $\dot{g}(x) = \frac{d}{dt}g(t,T_t(x))|_{t=0}$ 

the form

$$\begin{split} \frac{d}{dt} \int_{\Xi_t} g_t(y) dy|_{t=0} &= \int_{\Xi} [\dot{g}(x) + g(x)\vartheta'(x)] dx, \\ \frac{d}{dt} \int_{\Gamma_t} g_t(y) ds_y|_{t=0} &= \int_{\Gamma} [\dot{g}(x) + g(x)\theta'(x)] ds_x, \end{split}$$
  
where  $\vartheta'(x) &= \nabla \cdot V(x) \text{ and } \theta'(x) = \nabla \cdot V(x) - n(x)^\top \nabla V(x)^\top n(x). \end{split}$ 

Next we need to introduce transported differential operators. Let  $g_t \in H^k(\Xi_t)$ , if we think of  $\nabla_y g_t$  as a column vector, then the chain rule for derivatives gives

(3.9) 
$$(\nabla_y g_t(T_t(x)) = \mathfrak{T}_t^{-\top}(x) \cdot \nabla_x g_t := \mathfrak{N}^t(x) g^t,$$

where  $\mathfrak{N}_t(x)$  can be considered as the transported  $\nabla$ -operator. Eventually diminishing the interval  $[0, \varepsilon_0)$ , we may assume

(3.10) 
$$K_V \varepsilon_0 =: \|\nabla_x V; L^\infty(\mathbb{R}^3)\| \varepsilon_0 < 1$$

Since  $\mathfrak{T} = \mathbb{I} + t \nabla_x V$ , where  $\mathbb{I}$  is the  $3 \times 3$  unit matrix, we have

(3.11) 
$$\mathfrak{T}_t^{-\top}(x) = \sum_{\nu=0}^{\infty} (-1)^k t^k (\nabla_x V(x)^{\top})^k, \quad |t| \leq \varepsilon_0$$

Interchanging differentiation and summation, elementary calculations show

(3.12) 
$$\|\mathfrak{T}_t^{-\top}; L^{\infty}\| \leqslant \frac{1}{1 - \varepsilon_0 K_V}$$

(3.13) 
$$\|\nabla_x \mathfrak{T}_t^{-\top}; L^{\infty}\| \leq \frac{1}{(1-\varepsilon_0 K_V)^2} \|\nabla V; L^{\infty}\|,$$

(3.14) 
$$\|\nabla_x^2 \mathfrak{T}_t^{-\top}; L^{\infty}\| \leqslant C \left(\frac{\|\nabla V; L^{\infty}\|^2}{(1-\varepsilon_0 K_V)^3} + \frac{\|\nabla^2 V; L^{\infty}\|}{(1-\varepsilon_0 K_V)^2}\right),$$

here C is an absolut constant independent of V and t. The relations (3.9) and (3.11) imply

(3.15) 
$$\nabla_y g_t \circ T_t = \left( \mathbb{I} - t (\nabla_x V)^\top + t^2 ((\nabla_x V)^\top)^2 \mathfrak{T}_t^{-\top} \right) \cdot \nabla_x g^t.$$

3.4. The transported transmission problem. Now we return back to our transmission problem (2.6) – (2.8). Let  $\Omega$ ,  $\Omega^{\bullet}$  and  $\Gamma$  be defined as in Section 2.1, again  $\Gamma$  of class  $C^{2,\alpha}$  at least. We fix V and  $T_t$  as as in Section 3.3, then  $\Gamma_t = T_t\Gamma$  is of class  $C^{2,\alpha}$  for all  $t \in [0, \epsilon_0)$ . In addition to the assumptions of Section 2.1 on the Hooke matrices  $A^{\bullet}(x)$ ,  $A(x) = A^0 + A^e(x)$ , we require now  $A^{\bullet}, A^e \in C_0^1(\mathbb{R}^3)$ , and  $A^{\bullet}(x)$  is positive definit on a compact subset  $K \subset \mathbb{R}^3$ , which contains  $\bigcup_{t \in [0, \epsilon_0)} \Omega_t^{\bullet}$ . To the matrix differential operator  $D(\nabla_y)$  we associate the transported operator  $D_t(x, \nabla_x) =: D(\mathfrak{N}_t(x))$ . With

$$\mathbf{A}^t = A \circ T_t, \quad A^{\bullet,t} = A^{\bullet} \circ T_t$$

we define the transported elasticity operators on  $\Omega$ ,  $\Omega^{\bullet}$  by

(3.16) 
$$\mathcal{L}^{(\bullet),t}(x,\nabla_x) = -D^t(x,\nabla_x)^\top A^{(\bullet),t} D^t(x,\nabla_x)$$

Note that  $\mathcal{L}^t$ ,  $\mathcal{L}^{\bullet,t}$  are second order differential operators with variable coefficients which can be applied to any  $\{u, u^{\bullet}\} \in V^2_{\beta}(\Omega) \times H^2(\Omega^{\bullet})$ . In a similar manner, we introduce transported boundary operators. By  $\mathcal{N}_t$  and  $\mathcal{N}_t^{\bullet}$ , we denote the Neumann operators associated with the problem (2.6) – (2.8) on  $\Omega_t$ ,  $\Omega_t^{\bullet}$ . For  $x \in \Gamma$ ,  $y = T_t x \in \Gamma_t$ , let n(x) and  $n_t(y)$  be unit normal vectors in x and y (with the same orientation) to  $\Gamma$  and  $\Gamma_t$ , respectively. Then it holds (see [55, Sect. 2.17])

(3.17) 
$$n^{t}(x) := n_{t}(T_{t}(x)) = \left|\mathfrak{T}_{t}^{-\top} \cdot n(x)\right|^{-1}\mathfrak{T}_{t}^{-\top} \cdot n(x),$$

and we set

(3.18) 
$$\mathcal{N}_t^{(\bullet)} = D^\top (n^t(x)) \cdot A^{(\bullet),t}(x) D^t(x, \nabla_x)$$

The particular representations (3.11) and (3.15) enables us to control the behavior of the operators (3.16) and (3.18) at t = 0. To formulate our results, we introduce the following natural spaces for the data and for strong solutions to our transmission problems:

(3.19) 
$$\begin{aligned} \mathscr{D}_t &= V_1^2(\Omega_t)^3 \times H^2(\Omega_t^{\bullet})^3, \\ \mathscr{R}_t &= V_1^0(\Omega)^3 \times L^2(\Omega^{\bullet})^3 \times H^{3/2}(\Gamma_t)^3 \times H^{1/2}(\Gamma_t)^3, \end{aligned}$$

and the operators related to the transmission problems

$$(3.20) \qquad \mathscr{A}_t: \mathscr{D}_t \to \mathscr{R}_t, (u, u^{\bullet}) \mapsto (\mathcal{L}u, \mathcal{L}^{\bullet}u^{\bullet}, (u - u^{\bullet})|_{\Gamma_t}, (\mathcal{N}_t u - \mathcal{N}_t^{\bullet}u^{\bullet})|_{\Gamma_t}).$$

To the transported operators (3.16) and (3.18) we relate the problem operator  $\mathscr{A}_t$ . For t = 0, we simply write  $\mathscr{D}, \mathscr{R}$  and  $\mathscr{A}$ .

**Lemma 3.4.** Let V,  $T_t$  be defined as in Section 3.3, and  $t \in [0, \varepsilon_0]$ , so that  $T_t$  is a diffeomorphism and (3.10) holds.

- (i) The mapping I<sub>t</sub> : (u, u<sup>•</sup>) → (u<sub>t</sub>, u<sup>•</sup>) = (u ∘ T<sub>t</sub>, u<sup>•</sup> ∘ T<sub>t</sub>) defines a bounded isomorphism between D<sub>t</sub> and D. The norm of I<sub>t</sub> as well as the norm of the inverse I<sup>t</sup> is bounded independent of t. An analogous result holds for the spaces R<sub>t</sub> and R.
- (ii) To each set of data  $F_t = (f_t, f_t^{\bullet}, g_{0,t}, g_{1,t}) \in \mathscr{R}_t$  there exists a unique solution  $U_t = (u_t, u_t^{\bullet}) \in \mathscr{D}_t$  to the problem  $\mathscr{A}_t U_t = F_t$ , and

$$||U_t; \mathcal{D}_t|| \leq C_t ||F_t; \mathcal{R}_t||.$$

- (iii) If  $\mathscr{A}_t U_t = F_t$ , where  $U_t \in \mathscr{D}_t$ , and  $F_t \in \mathscr{R}_t$ , then by (i),  $U^t \in \mathscr{D}$ ,  $F^t \in \mathscr{R}$ , and  $\mathscr{A}^t U^t = F^t$ , in particular for  $t \in [0, \varepsilon_0)$ , the mapping  $\mathscr{A}^t$  is a bounded isomorphism from  $\mathscr{D}$  to  $\mathscr{R}$ .
- (iv) Let  $\mathscr{L}(\mathscr{D},\mathscr{R})$  denote the space of bounded linear operators from  $\mathscr{D}$  to  $\mathscr{R}$ , provided with the usual operator norm. The mapping  $t \mapsto \mathscr{A}^t$  is continuous from  $[0, \varepsilon_0)$  to  $\mathscr{L}(\mathscr{D}, \mathscr{R})$ , in particular we have  $\lim_{t \downarrow 0} \mathscr{A}^t = \mathscr{A}$ .

**Proof.** The first assertion follows from the representation (3.9), the estimates (3.12) - (3.14) and the transformation formula (3.8). Part (ii) follows from Proposition 2.3 together with local regularity results [54] and [49, Sect. 4.3].

For the proof of (iii) we observe that the definition of the transformed operators and functions immediately imply the equation  $\mathscr{A}^t U^t = F^t$ . The isomorphism property follows from part (i) and (ii) since  $\mathscr{A}^t = I^t \circ \mathscr{A}_t \circ I_t$ , where the mappings  $I_t : \mathscr{D} \to \mathscr{D}_t$  and  $I^t : \mathscr{R}_t \to \mathscr{R}$  are defined by  $I_t U = (u \circ T_t^{-1}, u^{\bullet} \circ T_t^{-1})$  and  $I^t F_t = F^t$ .

Turning to (iv), we first prove the continuity result. Obviously the mapping  $t \to T_t$  is in  $C^{\infty}([0,\tau]; C_0^3(\mathbb{R}^3))$  even for any large  $\tau > 0$ . Since  $A^{\bullet} \in C^1(K)$ , we obtain then for  $t, t_0 \in [0, \varepsilon_0)$ 

(3.21) 
$$\|A^{\bullet,t_0} - A^{\bullet,t}; L^{\infty}(K)\| + \|\nabla (A^{\bullet,t_0} - A^{\bullet,t}); L^{\infty}(K)\| \to 0,$$

similarly, since  $A(x) = A^0 + A^e(x)$ 

(3.22) 
$$||A^{t_0} - A^t; L^{\infty}(\mathbb{R}^3)|| + ||\nabla (A^{t_0} - A^t); L^{\infty}(\mathbb{R}^3)|| \to 0, \text{ as } t \to t_0.$$

The representation (3.15) gives

(3.23) 
$$Dt(x, \nabla_x) = D(\nabla_x) - tD((\nabla_x V)^\top \nabla_x) + t^2 \tilde{D}(t, x, \nabla_x),$$
$$\tilde{D}(t, x, \nabla_x) = \sum_{\nu=2}^{\infty} (-1)^{\nu} t^{\nu-2} D(((\nabla V)^\top)^k \nabla_x).$$

This means that  $\tilde{D}(t, x, \nabla_x)$  is a first order (matrix) differential operator, where the coefficient functions are bounded in  $C^2(\mathbb{R}^3)$  uniformly in t and vanish for large x, say  $|x| > R_0$ . Representation (3.23) implies that the mapping  $t \to D_t \in$  $\mathscr{L}(V_{\beta}^k(\Omega), V_{\beta}^{k-1}(\Omega))$  as well as  $t \to D_t \in \mathscr{L}(H^k(\Omega^{\bullet}), H^{k-1}(\Omega^{\bullet}))$  for  $k = 1, 2, \beta \in \mathbb{R}$ , is even Frechet-differentiable for all  $t \in [0, \varepsilon_0)$ , where the derivative is just the operator  $D((\nabla_x V)^\top \nabla)$  acting between the corresponding Sobolev spaces. Furthermore, representation (3.17) shows that again for small t, the vector fields  $n_t, \partial_t n_t \in C^2(\Gamma)$  and depend continuously on t. From here the continuity assertion follows using (3.21), (3.22).

We now assume that the data for the problem on the t-dependent domains are generated by restrictions of fixed vector fields, then Lemma 3.4 leads to the following result.

Corollary 3.5. For given

$$(3.24) f^{\bullet} \in L^{2}(\mathbb{R}^{3})^{3}, \quad f \in V_{1}^{0}(\mathbb{R}^{3})^{3}, \quad G^{0} \in H^{2}(\mathbb{R}^{3})^{3}, \quad G^{1} \in H^{1}(\mathbb{R}^{3})^{3}$$

we set

(3.25) 
$$f_t = f|_{\Omega_t}, \quad f_t^{\bullet} = f^{\bullet}|_{\Omega_t^{\bullet}}, \quad g_{0,t} = G^0|_{\Gamma_t}, \quad g_{1,t} = G^1|_{\Gamma_t}.$$

Let  $\mathcal{U}_t := \{u_t, u_t^{\bullet}\}$  and  $U = \{u, u^{\bullet}\}$  be the corresponding solution to problem (2.6) - (2.8) on  $\{\Omega_t, \Omega_t^{\bullet}, \Gamma_t\}$ , and  $\{\Omega, \Omega_{\bullet}, \Gamma\}$ , respectively, further  $\mathcal{U}^t := \{u^t, u^{\bullet, t}\}$  denote the transported vector field according to (3.3). Then  $\lim_{t \downarrow 0} U^t = U$  strongly in  $\mathcal{D}$ , *i.e.* 

$$||u^t - u; V_1^2(\Omega)|| + ||u^{\bullet,t} - u^{\bullet}; H^2(\Omega)|| \to 0, \text{ as } t \to 0.$$

**Proof.** With  $F^t$  defined by the data (3.25) we have  $F^t \to F = F_0$  strongly in  $\mathscr{R}$ . Part (iv) of Lemma 3.4 implies  $\mathscr{A}^{t,-1}$  converges to  $\mathscr{A}^{-1}$  in  $\mathscr{L}(\mathscr{R}, \mathscr{D})$ , hence

$$\begin{split} \|U^t - U; \mathscr{D}\| &= \|\mathscr{A}^{t, -1}F_t - \mathscr{A}^{-1}F; \mathscr{D}\| \\ &\leq \|\mathscr{A}^{t, -1}F^t - \mathscr{A}^{t, -1}F; \mathscr{D}\| + \|\mathscr{A}^{t, -1}F - \mathscr{A}^{-1}F; \mathscr{D}\| \to 0. \quad \Box \end{split}$$

On the other hand, the material derivatives are not really needed for the shape derivatives of the polarization tensor. Indeed, representation (2.42) shows that each entry of the polarization tensor is composed from two kinds of functionals. Recall that

$$\mathscr{Z}_{(k)} := \{Z_{(k)}, Z^{\bullet}_{(k)}\}, k = 1, \dots, 6,$$

is the solution to the transmission problem with data (2.36). The entries  $P_{kl}$  of the polarization tensor can be calculated as follows

(3.26) 
$$P_{kl} = \mathcal{P}_{kl} + 2a(\mathscr{Z}_{(k)}, \mathscr{Z}_{(l)}), \text{ where }$$

(3.27) 
$$\mathcal{P}_{kl} := -\int_{\Omega^{\bullet}} \left( A^0_{kl} - A^{\bullet}_{kl}(x) \right) dx + \int_{\Omega} A^e_{kl}(x)$$

(3.28)  
$$a(\mathscr{Z}_{(k)}, \mathscr{Z}_{(l)}) := -\frac{1}{2} (A(D(\nabla)Z_{(k)}, D(\nabla)Z_{(l)})_{\Omega} - \frac{1}{2} (A^{\bullet}(D(\nabla)Z_{(k)}^{\bullet}, D(\nabla)Z_{(l)}^{\bullet})_{\Omega^{\bullet}}.$$

Then term (3.27) is independent of  $\mathscr{Z}_{(k)}$  while *a* is an energy type functional. The energy for the field  $\mathscr{Z}_{(k)}$  is just  $a(\mathscr{Z}_{(k)}, \mathscr{Z}_{(k)})$ , and we can evaluate the off-diagonal elements of *P*, i.e.  $P_{kl}$  for  $k \neq l$ , by the formula

$$(3.29) \ 2a(\mathscr{Z}_{(k)}, \mathscr{Z}_{(l)}) = a(\mathscr{Z}_{(k)}, \mathscr{Z}_{(k)}) + a(\mathscr{Z}_{(l)}, \mathscr{Z}_{(l)}) - a(\mathscr{Z}_{(k)} - \mathscr{Z}_{(l)}, \mathscr{Z}_{(k)} - \mathscr{Z}_{(l)}) \ .$$

It means, that all the entries of the matrix P are can be calculated using Lemma 3.3 and the rules for derivatives of the energy functional. To this end we only need strong convergence of the minimizers as  $t \to 0$  which was shown in Corollary 3.5. If the data of the problem (2.6) - (2.8) are given through restrictions of sufficiently smooth data to the variable domains, then the methods of [55] for the first order shape sensitivity analysis can be applied. In the same way it is possible to prove the existence of strong material derivatives for the minimizers, which is here omitted, since for the the shape differentiability of the energy type functionals the strong convergence of unique minimizers is sufficient.

To determine the shape derivatives of the entries of polarization matrix, we first consider the entries on the diagonal, to this end we fix the index (k) and put

$$\mathscr{Z} := \mathscr{Z}_{(k)}$$

then  $\mathscr{Z}$  is the minimizer of the functional (3.1) for fixed interface  $\Gamma$ , where f and  $g^1$  are defined in (1.15). Let  $\Gamma_t$  be defined as in (3.2). Using the representation (3.26) and (3.27) with k = l, it comes down to find the shape derivative of

$$J(\Gamma) := 2a(\mathscr{Z}, \mathscr{Z}) := 2a(\mathscr{Z}_{(k)}, \mathscr{Z}_{(k)})$$

which we rewrite as follows (cf (1.15) and (3.1))

$$J(\Gamma) = a(\mathscr{Z}, \mathscr{Z}) - 2L(\mathscr{Z}) = \inf_{\mathfrak{v} \in V_0^1} [a(\mathfrak{v}, \mathfrak{v}) - 2L(\mathfrak{v})].$$

We repeat the same notation in the variable domain setting, hence

$$J(\Gamma_t) := 2a_t(\mathscr{Z}_t, \mathscr{Z}_t) = a_t(\mathscr{Z}_t, \mathscr{Z}_t) - 2L_t(\mathscr{Z}_t) = \inf_{\mathfrak{v}_t} [a_t(\mathfrak{v}_t, \mathfrak{v}_t) - 2L_t(\mathfrak{v}_t)].$$

To transport the minimized functional to the fixed domain, we replace simply the test functions  $\mathfrak{v}_t$  by test functions of a special form useful for our purpose, namely  $\mathfrak{v}_t := \mathfrak{u} \circ T_t^{-1}$ . In this way we get very simple expression to be differentiated

$$J(\Gamma_t) := \inf_{\mathfrak{u}} [a^t(\mathfrak{u},\mathfrak{u}) - 2L^t(\mathfrak{u})]$$

where  $a^t(\mathfrak{u},\mathfrak{u})$  and  $L^t(\mathfrak{u})$  are the forms transported to the fixed domain and interface, respectively. It is not difficult to find the derivatives with respect to t of the both forms, which we denote  $\dot{a}$  and  $\dot{L}$ , respectively. Thus, the energy functional is shape differentiable and we get the expression

$$dJ(\Gamma; V) = \dot{a}(\mathscr{Z}, \mathscr{Z}) - 2L(\mathscr{Z})$$

for its shape derivative. To be more precise, we get the shape derivatives of  $P_{kk}$  for all k. The expression of this particular form is already very useful for the numerical analysis, however, using the structure theorem we can also identify the boundary expression for the shape derivative, assuming the necessary regularity of the minimizers and of the interface.

The second step is just to extend the analysis of the shape differentiability for the arbitrary indices (k), (l) which can be performed in the same way in view of the formula (3.29). It means that we get exactly the same form of shape derivatives of all entries of the polarization matrix as for the entries on the diagonal with (k) = (l).

3.5. Energy matrix function. We denote by  $\mathbf{J}(\Gamma_t)$  the 6 × 6-matrix, where the entries  $J_{k,l}(\Gamma_t)$  are defined with the help of  $\mathscr{Z}_{t,(k)}$  in the perturbed domains, i.e.

$$(3.30) J_{k,l}(\Gamma_t) = \frac{1}{2} a_t(\mathscr{Z}_{t,(k)}, \mathscr{Z}_{t,(l)}) - L_t(\mathscr{Z}_{t,(l)}) = -\frac{1}{2} a_t(\mathscr{Z}_{t,(k)}, \mathscr{Z}_{t,(l)}) = \\ = \frac{1}{2} (AD(\nabla)Z_{t,(k)}, D(\nabla)Z_{t,(l)})_{\Omega_t} + \frac{1}{2} (A^{\bullet}D(\nabla)Z_{t,(k)}^{\bullet}, D(\nabla)Z_{t,(l)}^{\bullet})_{\Omega_t^{\bullet}} - \\ - (f_t, Z_{t,(l)})_{\Omega_t} - (f_t^{\bullet}, Z_{t,(l)}^{\bullet})_{\Omega_t^{\bullet}} - (g_t^1, Z_{t,(l)} = Z_{t,(l)}^{\bullet})_{\Gamma_t} = \\ - \frac{1}{2} (AD(\nabla)Z_{t,(k)}, D(\nabla)Z_{t,(l)})_{\Omega_t} - \frac{1}{2} (A^{\bullet}D(\nabla)Z_{t,(k)}^{\bullet}, D(\nabla)Z_{t,(l)}^{\bullet})_{\Omega_t^{\bullet}}$$

where  $f_t = f_{(l)} \circ T_t$ ,  $g_t^1 = g_{(l)}^1 \circ T_t$  and  $f_{(l)}$ ,  $g_{(l)}^1$  are taken from (2.36). Assuming for simplicity that the matrices  $A, A^{\bullet}$  are constant, we transport  $J_{k,l}(\Gamma_t)$  to the fixed domain which leads to the following expression

$$(3.31) J(\Gamma_t) = \frac{1}{2} a^t (\mathscr{Z}_{(k)}^t, \mathscr{Z}_{(l)}^t) - L^t (\mathscr{Z}_{(l)}^t) = -\frac{1}{2} a^t (\mathscr{Z}_{(k)}^t, \mathscr{Z}_{(l)}^t) = \\ = \frac{1}{2} (\vartheta(t) A D^t (\nabla) Z_{(k)}^t, D^t (\nabla) Z_{(l)}^t)_{\Omega} + \frac{1}{2} (\vartheta(t) A^{\bullet} D^t (\nabla) Z_{(k)}^{\bullet, t}, D^t (\nabla) Z_{(l)}^{\bullet, t})_{\Omega^{\bullet}} - \\ - (\theta(t) F^t, Z_{(l)}^t)_{\Omega} - (\theta(t) F_t^{\bullet}, Z_{(l)}^{\bullet, t})_{\Omega^{\bullet}} - (\theta(t) g^{1, t}, Z_{(l)}^t)_{\Gamma} = \\ - \frac{1}{2} (\vartheta(t) A D^t (\nabla) Z_{(k)}^t, D^t (\nabla) Z_{(l)}^t)_{\Omega} - \frac{1}{2} (\vartheta(t) A^{\bullet} D^t (\nabla) Z_{(k)}^{\bullet, t}, D^t (\nabla) Z_{(l)}^{\bullet, t})_{\Omega^{\bullet}} ,$$

where again  $D^t(\nabla) = D(\mathfrak{T}^{-\top}\nabla_x)$  according to the transformation rules. From Lemma 3.5 it follows that in the fixed domain setting we have the shape differentiability result.

**Proposition 3.6.** All entries  $J_{k,l}(\Gamma)$  of the matrix shape functional  $\mathbf{J}(\Gamma_t)$  are shape differentiable i.e., the following limits exist

(3.32) 
$$dJ_{k,l}(\Gamma; V) = \lim_{t \to 0} \frac{1}{t} (J_{k,l}(\Gamma_t) - J_{k,l}(\Gamma))$$

Furthermore, the Hadamard structure theorem of the shape gradient [55] implies the continuity of the mapping  $C_0^1(\mathbb{R}^3) \ni V \mapsto dJ_{k,l}(\Gamma; V) \in \mathbb{R}$ . Therefore, there are shape gradients  $\mathfrak{g}_{k,l}^{\Gamma}$  such that

(3.33) 
$$dJ_{k,l}(\Gamma; V) = \langle \mathfrak{g}_{k,l}^{\Gamma}, V \cdot n \rangle_{\Gamma}$$

in the duality pairing on the interface  $\Gamma$ .

The direct evaluation of the shape derivative  $dJ(\Gamma; V)$  leads to quite complicated expressions, however, explicit formulae are useful from the point of view of possible applications. We are going to present the formal time derivative at t = 0 of the energy functionals where we suppose regularity assumptions under which the surface integrals make sense,

$$dJ_{k,l}(\Gamma; V) := \frac{d}{dt} J_{k,l}(\Gamma_t) = \frac{1}{2} \int_{\Gamma} \{ (AD(\nabla)Z_{(k)}, D(\nabla)Z_{(l)}) - (A^{\bullet}D(\nabla)Z_{(k)}^{\bullet}, D(\nabla)Z_{(l)}^{\bullet}) \} V \cdot nds_x \\ (3.34) \qquad - \int_{\Gamma} (f - f^{\bullet}, Z_{(l)}) V \cdot nds_x - \int_{\Gamma} (\theta'(0)g^1 + (g^1)'_{\Gamma}), Z_{(l)}) V \cdot nds_x ,$$

where  $(g^1)'_{\Gamma}$  is the so-called boundary shape derivative [55] of the element  $g^1$ .

If there is no regularity required here, the shape derivative  $dJ(\Gamma; V)$  can be expressed in terms of material derivatives by volume integrals, and the structure theorem [55] can be used in order to obtain the boundary formula in the sense of distributions.

3.6. **Polarization tensor.** The shape differentiability of energy functionals implies the shape differentiability of the polarization tensor. From formula (2.42) we get for the perturbed interface

(3.35) 
$$P_t = -\int_{\Omega_t^{\bullet}} \left(A^0 - A^{\bullet}(x)\right) dx + \int_{\Omega_t} A^e(x) + 2\mathbf{J}(\Gamma_t) \ .$$

Therefore, the time derivative P' of the tensor  $P_t$  is given by the formula

(3.36) 
$$P' = -\int_{\Gamma} \left( A^0 - A^{\bullet}(x) + A^e(x) \right) V \cdot n ds_x + 2d \mathbf{J}(\Gamma; V) .$$

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