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ABSTRACT. Asymptotic formulae for the mechanical and electric fields in a piezoelectric body with a small void are derived and justified. Such results are new and useful for applications in the field of design of smart materials. In this way the topological derivatives of shape functionals are obtained for piezoelectricity. The asymptotic formulae are given in terms of the so-called polarization tensors (matrices) which are determined by the integral characteristics of voids. The distinguished feature of the piezoelectricity boundary value problems under considerations is the absence of positive definiteness of an differential operator which is non self-adjoint. Two specific Gibbs' functionals of the problem are defined by the energy and the electric enthalpy. The topological derivatives are defined in different manners for each of the governing functionals. Actually, the topological derivative of the enthalpy functional is local i.e., defined by the pointwise values of the governing fields, in contrary to the energy functional and some other suitable shape functionals which admit non-local topological derivatives, i.e., depending on the whole problem data. An example with the weak interaction between mechanical and electric fields provides the explicit asymptotic expansions and can be directly used in numerical procedures of optimal design for smart materials.

Keywords: Shape optimization, asymptotic analysis, piezoelectricity, electric enthalpy, topological derivative
MSC: Primary 35Q30, 49J20, 76N10; Secondary 49Q10, 74P15

1. INTRODUCTION

The paper is devoted to the asymptotic analysis of boundary value problems for coupled models. The coupling occurs between the mechanical part which takes the form of the linearized elasticity and governs the stress-strain state of the body, and the electrical part which describes the electromagnetic field in the body.

From the view point of applications, piezoelectric materials are of common use in electromechanical sensors and actuators, e.g., ultrasound transducers in medical imaging and therapy, force and acceleration sensors, positioning sensors, surface acoustic wave filters, still with the growing range of applications in modern technology. Their mode of action is based on the piezoelectric effect, that couples the electrical and mechanical behavior of such materials. For the optimal design of piezoelectric devices, efficient numerical procedures for shape and topology optimization should be still developed. In the modern theory of shape optimization it is required that the derivation of shape and topological derivatives of shape functionals to be optimized is performed beforehand. From one side, the derivation of shape gradients of integral functionals in smooth domains [45] and non-smooth domains

[25] (cf. [36, 37]) has become a standard procedure. There is no major difficulty to perform such a shape sensitivity analysis for the elliptic boundary value problem under considerations. However, the boundary value problem in piezoelectricity cannot be posed in such a way that it simultaneously is formally self-adjoint and possesses a semi-bounded quadratic form. This specific feature makes the problem more involved from the asymptotic analysis point of view compared to the pure elasticity or pure electricity boundary value problems. In addition, the general case of inhomogeneous and anisotropic body is considered, which also requires for additional and new technicalities in asymptotic procedures which is the main subject of the paper. In particular, different formulations of the piezoelectricity problem (cf. Sections 2.2, 2.3, 3.3) lead to two definitions of the polarization matrices which differ one from another by its properties. Moreover, only the electrical enthalpy, which is but the governing functional for the piezoelectric media (see, e.g., [11, 14, 42]) admits the topological derivative dependent on local characteristics of mechanical and electrical fields. Other shape functionals, especially the energy functional, get the topological derivatives dependent on the global characteristics of mechanical and electrical fields. This acquired trait raises the natural question on the properties of material derivatives for piezoelectricity in the framework of the shape sensitivity analysis with smooth or non-smooth boundary variations, it is clear that the result could be of the same nature, since the topological derivatives can be identified from the first order shape gradients by a limit passage e.g. in elasticity, [47] (cf. also [13]).

In the paper, we restrict ourselves to the asymptotic procedures of singular domain perturbations which allow us to obtain, in a natural way, the topological derivatives of shape functionals. In principle, the method developed here can be generalized to characterize the influence on solutions of the non-smooth boundary variations, therefore, we can derive the shape gradients even in such a case, e.g., for small defects located close-by the boundary, including micro-cracks (see [38]).

Without entering into details, but with the strong practical implications in mind, we can claim that some possible applications of shape optimization in the field concern the design of electro-acoustic transducers which are constructed with piezoelectric actuator-patches and capacitative micro-machined ultrasound transducers. The task for optimal design for a class of electrostatic-mechanical-acoustic transducers can be e.g., the topology of electro-acoustic material and the topology of the electrode-layers, in order to achieve a maximal acoustic pressure, or a maximal acoustic energy in a specific sub-domains of the hold-all-domain. We refer the reader e.g. to [42, 11, 14] for modeling of piezoelectric materials, to [16] for material tensor identification for such materials, and to [17] for control issues.

Our aim is a possible application in shape optimization, thus we introduce the so-called topological derivatives of shape functionals for piezoelectric materials. It seems that the models are not up to now used in applied mathematics for the purposes of shape optimization, although the smart materials are of common use in the engineering practice. In shape optimization, the modern approach to numerical solution, requires the preliminary knowledge of explicit formulae for shape gradients [45] as well as of the topological derivatives [46, 36, 9]. These formulae are used in the *level-set*-type methods which model the geometrical domain evolution by a zero-level set of solutions to non-linear hyperbolic equations of the Hamilton-Jacoby type. The shape gradient are present as the coefficients of the equations, and the topological derivatives are used to improve the values of the shape functional under consideration by the appropriate topology changes, e.g., for the minimization of the shape functional, the minima of the topological derivative of the functional indicate the location of a new hole in the geometrical domain [2, 7, 8].

2. Formulation of the problem and the preliminary description of results

2.1. **Shape optimization in piezoelectricity.** This paper is motivated by the fact that, among numerous publications on shape optimization, shape sensitivity analysis for piezoelectric bodies does not exist, although piezoelectric materials are of extremely wide usage in the modern technologies, one can think of a simple lighter, available in any supermarket, or an elaborated computer work-station in a university. One, and definitely not the only one, distinguishing feature of such smart materials implies an easy energy transfer in both directions from mechanical fields to electric fields. The mathematical modeling of such a phenomenon leads to serious complications of analysis for governing PDE's because the corresponding boundary value problem is not formally self-adjoint in contrast to the boundary value problems for purely elastic bodies or purely electromagnetic media. This fact requires for the development of new mathematical tools and a careful choice of the cardinal shape functional while neglecting of non-self-adjointness provokes mistakes in both, mathematical formulae and physical interpretation of the obtained results (see Remark 4.4 below).

Introduced in [46][1], the topological derivative $T(u^0;\omega_1)$ of a shape functional $\mathcal{J}$ is intended to describe the change of the functional $\mathcal{J}$ due to nucleation of holes or voids and allows to extend possible variations of the shape in an optimization process [2, 7, 8] in comparison with classical tools (cf. [45, 4, 5]),

$$\mathcal{J}(u^h;\Omega(h)) = \mathcal{J}(u;\Omega) + h^{\kappa}\mathcal{T}(u;\omega_1) + o(h^{\kappa}),\ h \to +0, \tag{1}$$

In (1), $h > 0$ is a small parameter, i.e., the diameter of the opening ω_h in the entire body $\Omega \subset \mathbb{R}^n$, u^h and u are solutions of the boundary value problem in $\Omega(h) = \Omega \setminus \overline{\omega}_h$ and Ω, respectively, and the exponent $\kappa > 0$ depends on the space dimension n and boundary conditions imposed on the interior $(n-1)$-dimensional surface $\partial\omega_h$.

Asymptotic analysis of elliptic problems in singularly perturbed domains, e.g., methods of matched and compound asymptotic expansions (cf. [15] and [25], respectively), has become the most appropriate and relevant to obtain *almost explicit* formulae for the topological derivatives as it has been demonstrated in [36, 37] and others. We also mention books [28, 3] where the subject is studied, to some extend, from physical and numerical point of view.

[1]Actually, asymptotic formulae of type (1) together with the whole asymptotic series for energy functionals under various singular boundary perturbations had been derived much earlier in [24], although the notion of the topological derivative is due to [46].

Strangely enough, only self-adjoint problems were heretofore examined carefully, although the full-blown approach in [25] can work for general boundary value problems for elliptic systems. In this paper we partly fill this gap by adapting formula (1) to certain shape functionals for a piezoelectric body.

The piezoelectricity problems admits two different formulations with non-symmetric and symmetric but non-semibounded quadratic forms, the energy and electric enthalpy functionals, respectively. By means of the Lax-Milgram lemma, the first formulation furnishes the existence and uniqueness result. At the same time, the topological derivative of the energy functional is a non-local characteristics of the piezoelectricity solutions in contrast to the pure elasticity problem (see Remark 4.3 below), while the absence of this intrinsic property is not caused by an *incorrect* definition (1) but occurs as well for the energy release rate in mechanics of cracks for piezoelectric media (see Remark 4.3 again). The fair explanation, we refer the reader to [48] for the modeling issues, of the latter refers to the electric enthalpy as one of Gibbs' functional obtained from the energy functional by the partial Lagrange transform on the electric components. This is the electric enthalpy $\mathcal{E}(u^h;\Omega(h))$ (see the definition in (20)), that governs the mechanical electric state of the piezoelectric body $\Omega(h)$ and, therefore, the second formulation becomes variational and provides the clear interpretation of the topological derivative $\mathcal{T}_{\mathcal{E}}(u;\omega_1)$ in

$$\mathcal{E}(u_h;\Omega(h)) = \mathcal{E}(u;\Omega) + h^3\mathcal{T}_{\mathcal{E}}(u;\omega_1) + O(h^4),\ h \to +0. \tag{2}$$

The indicated peculiarity of the piezoelectricity problem crucially influences topological derivatives of other shape functionals, too. For example, the traditional adjoint state (cf. [4, 45, 46]) has to be found out in the formally adjoint boundary value problem that occasionally underlines its name.

All the above observations lifts the piezoelectricity problem on the top of the list of unsolved problems in shape optimization, it seems that even the classical formulae for material derivatives, which are not under consideration in the paper, ought to be revisited.

2.2. **Constitutive relations in piezoelectricity.** Let $\Omega \subset \mathbb{R}^3$ be a piezoelectric body with the Lipschitz boundary $\partial\Omega$ and the compact closure $\overline{\Omega} = \Omega \cup \partial\Omega$. Using the matrix/column notation (cf. [22, 29]), we regard the displacement vector u^{M} as the column $u^{\mathsf{M}} = (u^{\mathsf{M}}_1, u^{\mathsf{M}}_2, u^{\mathsf{M}}_3)^\top$ where u^{M}_j is the projection of u on the x_j-axis of the fixed Cartesian coordinates system $x = (x_1, x_2, x_3)^\top$ and $\top$ stands for transposition. Together with the electric potential u^{M}, the displacements compose the column $u = (u^{\mathsf{M}}_1, u^{\mathsf{M}}_2, u^{\mathsf{M}}_3, u^{\mathsf{E}})^\top$ of height 4. The strain column

$$\varepsilon^{\mathsf{M}}(u^{\mathsf{M}}) = (\varepsilon^{\mathsf{M}}_{11}, \varepsilon^{\mathsf{M}}_{22}, \varepsilon^{\mathsf{M}}_{33},\ \sqrt{2}\varepsilon^{\mathsf{M}}_{23},\ \sqrt{2}\varepsilon^{\mathsf{M}}_{31},\ \sqrt{2}\varepsilon^{\mathsf{M}}_{12})^\top \tag{3}$$

consists of the Cartesian components $\varepsilon^{\mathsf{M}}_{jk} = \frac{1}{2}(\partial_j u^{\mathsf{M}}_k + \partial_k u^{\mathsf{M}}_j)$ of the strain tensor and takes the form $\varepsilon^{\mathsf{M}}(u^{\mathsf{M}}) = D^{\mathsf{M}}(\nabla_x)u^{\mathsf{M}}$ where

(4)
$$D^{\mathsf{M}}(\nabla_x)^\top = \begin{pmatrix} \partial_1 & 0 & 0 & 0 & 2^{-1/2}\partial_3 & 2^{-1/2}\partial_2 \\ 0 & \partial_2 & 0 & 2^{-1/2}\partial_3 & 0 & 2^{-1/2}\partial_1 \\ 0 & 0 & \partial_3 & 2^{-1/2}\partial_2 & 2^{-1/2}\partial_1 & 0 \end{pmatrix}, \nabla_x = \begin{pmatrix} \partial_1 \\ \partial_2 \\ \partial_3 \end{pmatrix}, \partial_j = \frac{\partial}{\partial x_j}.$$

We introduce the column $\varepsilon(u) = (\varepsilon^{\mathsf{M}}(u^{\mathsf{M}})^\top, \varepsilon^{\mathsf{E}}(u^{\mathsf{E}})^\top)^\top$ where $\varepsilon^{\mathsf{E}}(u^{\mathsf{E}}) = \nabla_x u^{\mathsf{E}}$ is the electric strain column, taken with the sign minus, and $D(\nabla_x)$ implies a (9×4)-matrix of the first-order differential operators,

$$\varepsilon(u) = D(\nabla_x)u,\ D(\nabla_x)^\top = \begin{pmatrix} D^{\mathsf{M}}(\nabla_x)^\top & \mathbf{0} \\ \mathbf{0}\quad\mathbf{0} & \nabla_x^\top \end{pmatrix},\ \mathbf{0} = (0,0,0). \tag{5}$$

We also assemble the column $\sigma(u)$ of height 9 from the stress column $\sigma^{\mathsf{E}}(u^{\mathsf{M}})$ of structure (3) and the electric induction column $\sigma^{\mathsf{E}}(u^{\mathsf{E}}) = (\sigma^{\mathsf{E}}_1, \sigma^{\mathsf{E}}_2, \sigma^{\mathsf{E}}_3)^\top$. In this manner, the constitutive relations of piezoelectricity (see [11, 14, 42])

$$\sigma^{\mathsf{M}} = A^{\mathsf{MM}}\varepsilon^{\mathsf{M}} - A^{\mathsf{ME}}\varepsilon^{\mathsf{E}},\ \sigma^{\mathsf{E}} = A^{\mathsf{EM}}\varepsilon^{\mathsf{M}} + A^{\mathsf{EE}}\varepsilon^{\mathsf{E}} \tag{6}$$

can be rewritten as follows:

$$\sigma(u) = A\varepsilon(u), \tag{7}$$

where the matrix A of size 9×9,

$$A = \begin{pmatrix} A^{\mathsf{MM}} & -A^{\mathsf{ME}} \\ A^{\mathsf{EM}} & A^{\mathsf{EE}} \end{pmatrix} \tag{8}$$

is formed by the symmetric and positive definite (6×6)- and (3×3)-matrices A^{MM} and A^{EE}, respectively the elastic stiffness matrix and the dielectric permeability matrix, and the blocks $A^{\mathsf{ME}} = (A^{\mathsf{EM}})^\top$ of piezoelectric moduli. We emphasize that, by its physical nature, the matrix (8) is not symmetric provided the (6×3)-block A^{ME} is not null, i.e., the mechanical and electric fields interact.

The state of the piezoelectric body Ω is described by the mixed boundary value problem

$$D(-\nabla_x)^\top A(x) D(\nabla_x)u(x) = f(x),\ x \in \Omega, \tag{9}$$

$$D(n(x))^\top A(x) D(\nabla_x)u(x) = g(x),\ x \in \Gamma_\sigma, \tag{10}$$

$$u(x) = 0,\ x \in \Gamma_u = \partial\Omega \setminus \overline{\Gamma}_\sigma, \tag{11}$$

where $n = (n_1, n_2, n_3)^\top$ is the unit vector (column) of the outward normal. On the right hand-side of the equations (9) and (10), we have the volume forces $f^{\mathsf{M}} = (f^{\mathsf{M}}_1, f^{\mathsf{M}}_2, f^{\mathsf{M}}_3)^\top$ and the surface mechanical loading $g^{\mathsf{M}} = (g^{\mathsf{M}}_1, g^{\mathsf{M}}_2, g^{\mathsf{M}}_3)^\top$ together with the volume f^{E} and surface g^{E} electric charges. The Dirichlet conditions (11) mean that the body is mechanically clamped over the surface Γ_u and in contact with an electric conductor. As usually, $f^{\mathsf{E}} = 0$ and, if the surface Γ_σ is in contact with a dielectric medium, i.e., vacuum, we are to put $g^E_4 = 0$.

2.3. **Solvability of the problem.** Let us assume that $mes_2\Gamma_u > 0$ and $f \in L^2(\Omega)^4$, $g \in L^2(\Gamma_\sigma)^4$ where $L^2(\Xi)$ denote the Lebesque space with the intrinsic inner product $(\ ,\ )_\Xi$ and the superscript 4 indicates the number of components in the vector functions f and g. Notice that the subscript is always omitted in our notation for inner products and norms.

The integral identity (cf. [21]) serving for problem (9)-(11), reads as follows:

$$Q(u, v; \Omega) := (AD(\nabla_x)u, D(\nabla_x)v)_\Omega = (f, v)_\Omega + (g, v)_{\Gamma_u},\ v \in \mathring{H}^1(\Omega; \Gamma_u)^4, \tag{12}$$

where $\mathring{H}^1(\Omega; \Gamma_u)$ denotes the Sobolev space of functions vanishing at Γ_u. The left-hand side of (12) is understood properly provided entries of the matrix A are measurable and uniformly bounded functions in Ω. In addition, for almost all $x \in \Omega$, we assume the symmetry and positivity properties

$$\begin{aligned} &A^{\mathsf{MM}}(x) = A^{\mathsf{MM}}(x)^\top,\ A^{\mathsf{ME}}(x) = A^{\mathsf{ME}}(x)^\top,\ A^{\mathsf{EE}}(x) = A^{\mathsf{EE}}(x)^\top,\\ &c_{\mathsf{M}}|a^{\mathsf{M}}|^2 A^{\mathsf{MM}}(x)a^{\mathsf{M}} \le C_{\mathsf{M}}|a^{\mathsf{M}}|^2,\ a^{\mathsf{M}} \in \mathbb{R}^6,\\ &c_{\mathsf{E}}|a^{\mathsf{E}}|^2 A^{\mathsf{EE}}(x)a^{\mathsf{E}} \le C_{\mathsf{E}}|a^{\mathsf{E}}|^2,\ a^{\mathsf{E}} \in \mathbb{R}^6, \end{aligned} \tag{13}$$

where c_{M}, C_{M} and c_{E}, C_{E} are positive constants. We emphasize that no positivity restriction is imposed on the piezoelectric moduli in A^{ME}.

Although in the case $A^{\mathsf{ME}} \neq 0$ the sesquilinear form $Q(\cdot, \cdot; \Omega)$ cannot be an inner product on the Hilbert space $\mathring{H}^1(\Omega; \Gamma_u)^4$ due to the *wrong* sign on A^{ME} in (8), the Lax-Milgram lemma ensures the following assertion because of the formula

$$Q(u, u; \Omega) = (A^{\mathsf{MM}}D^{\mathsf{M}}(\nabla_x)u^{\mathsf{M}}, D^{\mathsf{M}}(\nabla_x)u^{\mathsf{M}})_\Omega + (A^{\mathsf{EE}}\nabla_x u^{\mathsf{E}}, \nabla_x u^{\mathsf{E}})_\Omega \ge c\|u; H^1(\Omega)\|^2 \tag{14}$$

caused by the Poincaré inequality for u^{E} and the Korn inequality for u^{M} (see [6, 19] and others).

Proposition 2.1. *Under the conditions* (13), (14), *the problem* (12) *admits a unique solution* $u \in \mathring{H}^1(\Omega; \Gamma_u)^4$, *and the following estimate is valid:*

$$\|u; H^1(\Omega)\| \le c_\Omega(\|f; L^2(\Omega)\| + \|g; L^2(\Gamma_\sigma)\|). \tag{15}$$

Unfortunately, the problem (12) is non variational. Indeed, the energy functional $\mathcal{U}$,

$$\mathcal{U}(u; \Omega) = \frac{1}{2}(AD(\nabla_x)u, D(\nabla_x)u)_\Omega - \mathcal{A}(u; \Omega), \tag{16}$$

$$\mathcal{A}(u; \Omega) := (f, u)_\Omega + (g, u)_{\Gamma_\sigma}, \tag{17}$$

is but the sum of the mechanical and electric energy functionals

$$\mathcal{U}^{\mathsf{M}}(u^{\mathsf{M}}; \Omega) = \frac{1}{2}(A^{\mathsf{MM}}D^{\mathsf{M}}(\nabla_x)u^{\mathsf{M}}, D^{\mathsf{M}}(\nabla_x)u^{\mathsf{M}})_\Omega - (f^{\mathsf{M}}, u^{\mathsf{M}})_\Omega - (g^{\mathsf{M}}, u^{\mathsf{M}})_{\Gamma_\sigma}, \tag{18}$$

$$\mathcal{U}^{\mathsf{E}}(u^{\mathsf{E}}; \Omega) = \frac{1}{2}(A^{\mathsf{EE}}\nabla_x u^{\mathsf{E}}, \nabla_x u^{\mathsf{E}})_\Omega - (f^{\mathsf{E}}, u^{\mathsf{E}})_\Omega - (g^{\mathsf{E}}, u^{\mathsf{E}})_{\Gamma_\sigma}, \tag{19}$$

while a stationary point of (16) becomes a solution of the problem (12) with the block-diagonal (9×9)-matrix $diag\{A^{\mathsf{MM}}, A^{\mathsf{EE}}\}$, i.e., the variational problem does not accept an interaction of the mechanical and electric fields (cf. an example in Section 4.4).

It is known (see, e.g., [48]) that the electric enthalpy $\mathcal{E}$,

$$\mathcal{E}(u;\Omega) = \frac{1}{2}(A_{(-)}D(\nabla_x)u, D(\nabla_x)u)_\Omega - \mathcal{R}(u;\Omega), \tag{20}$$

$$\mathcal{R}(u;\Omega) = (f^{\mathsf{M}}, u^{\mathsf{M}})_\Omega + (g^{\mathsf{M}}, u^{\mathsf{M}})_{\Gamma_\sigma} - (f_4^{\mathsf{E}}, u_4^{\mathsf{E}})_\Omega - (g_4^{\mathsf{E}}, u_4^{\mathsf{E}})_{\Gamma_\sigma}, \tag{21}$$

gives rise to the variational formulation of the piezoelectricity problem

$$Q_{(-)}(u,v;\Omega) := (A_{(-)}D(\nabla_x)u, D(\nabla_x)v)_\Omega = \mathcal{R}(v;\Omega),\ v \in \mathring{H}^1(\Omega;\Gamma_\sigma)^4, \tag{22}$$

where the matrix $A_{(-)}$ is composed from blocks in (8) as follows

$$A_{(-)} = \begin{pmatrix} A^{\mathsf{MM}} & A^{\mathsf{ME}} \\ A^{\mathsf{EM}} & -A^{\mathsf{EE}} \end{pmatrix} \tag{23}$$

The matrix (23), in contrast to the matrix A, is symmetric, however, neither matrix (23), nor the quadratic form on the left-hand side of (22) is positive definite. Thus, a solution $u \in \mathring{H}^1(\Omega;\Gamma_\sigma)^4$ is a stationary point of the functional (20) but u cannot be any minimizer of the electric enthalpy $\mathcal{E}(u;\Omega)$.

The integral identity (22) with the test function $v_{(-)} = (v_1^{\mathsf{M}}, v_2^{\mathsf{M}}, v_3^{\mathsf{M}}, -v^{\mathsf{E}})$ transforms into the problem (12). The inverse transformation is also available. These facts prove that the problem (22) inherits the unique solvability from (12) in Proposition 2.1.

Remark 2.1. *The integral identity is formally obtained by the multiplying system* (9) *with v scalarly and integrating by parts. Using $v_{(-)}$ as the multiplier, one arrives at* (22). *This explains the equivalency of the problems. In Section 3.3 we shall outline a different way to modify the piezoelectricity problem in order to study properties of the mechanical and electric fields on the base of known results.*

The electric enthalpy is but the difference of elastic energy (18) and electric energy (19). Expression (17) implies the external work. Being the difference of the mechanical and electric external works, the component $\mathcal{R}(u;\Omega)$ of the electric enthalpy has no physical meaning as a whole. Nevertheless, in Section 4.2 we shall observe that asymptotic formulae for $\mathcal{E}(u;\Omega)$ become meaningful while the analogous formulae for $\mathcal{U}(u;\Omega)$ look rather queer.

2.4. **Structure of the paper.** In Section 3 the asymptotic analysis of the piezoelectricity problem for the body $\Omega(h)$ with a small void $\overline{\omega_h}$ is performed (see (24)). The applied here asymptotic procedure [25, Ch.4] requires for introduction of an intrinsic integral characteristics of the void $\overline{\omega_1}$ in the homogeneous piezoelectric space $\mathbb{R}^3$, the polarization matrix $M(A^0,\omega)$ of size 9×9 (see formulae (61)-(63)). Theorem 3.4 establishes general properties of the polarization matrix, see also (172) for the case of weak interaction between mechanical and electric fields. The polarization matrix appears in the asymptotic expansion of the boundary layer term at infinity that also permits in Section 3.5 to complete the asymptotic ansatz of the solution to the piezoelectricity problem in $\Omega(h)$. The asymptotics constructed in Section 3 is justified in section 4.1. In Section 4.2 the asymptotics of the energy and electric enthalpy functionals are analysed, while in Section 4.3 rather arbitrary shape functional is considered and the corresponding adjoint state is detected. The paper is completed by inquiring into a piezoelectric body with a weak interaction of the mechanical and electric fields. All asymptotic formulae derived in the paper are made more explicit in such a case due to the fact that for pure electricity and pure elasticity the polarization matrices are known explicitly for many canonical shapes (see, respectively, [44], [49, 23, 3] and others).

3. Asymptotic analysis

3.1. **The problem with an interior singular perturbation in the domain.** Let ω be an open set in $\mathbb{R}^3$ with a Lipschitz boundary and a compact closure. We assume that both Ω and ω contain the coordinate origin $\mathcal{O}$. Given a small dimensionless parameter $h \in (0, h_0]$, we introduce the sets

$$\omega_h = \{x : \xi := h^{-1}x \in \omega\},\ \Omega(h) = \Omega \setminus \overline{\omega_h}. \tag{24}$$

The bound $h_0 > 0$ is chosen such that $\overline{\omega_h} \subset \Omega$ for $h \in (0, h_0]$. By rescaling, we reduce a characteristic size of Ω and ω to the unit and make the coordinates x and ξ dimensionless.

Supposing $\Omega(h)$ to be a connected set, we consider the piezoelectricity problem in the domain $\Omega(h)$, namely,

$$D(-\nabla_x)^\top A(x)D(\nabla_x)u^h(x) = f(x),\ x \in \Omega(h), \tag{25}$$

$$D(n(x))^\top A(x)D(\nabla_x)u^h(x) = g(x),\ x \in \Gamma_\sigma, \tag{26}$$

$$D(n^h(x))^\top A(x)D(\nabla_x)u^h(x) = 0,\ x \in \partial\omega_h, \tag{27}$$

$$u^h(x) = 0,\ x \in \Gamma_u. \tag{28}$$

In (27), n^h stands for the outward normal on $\partial\omega_h$. Since the Neumann conditions are imposed on the boundary of ω_h, there is no traction on $\partial\omega_h$ and the opening $\overline{\omega_h}$ is filled with a dielectric medium. This problem, of course, ought to be reformulated as either integral identity (12), or (22) in the function space $\mathring{H}^1(\Omega(h); \Gamma_u)^4$, hence

$$Q(u^h, v^h; \Omega(h)) = (f, v^h)_{\Omega(h)} + (g, v^h)_{\Gamma_\sigma},\ v^h \in \mathring{H}^1(\Omega(h); \Gamma_u)^4. \tag{29}$$

Proposition 2.1 remains valid for the problem (29) in the domain $\Omega(h)$.

For $h = 0$, the opening ω_h disappears and the singularly perturbed problem (25)-(28) becomes the original problem (9)-(11). In order to describe the behavior of the solution $u^h \in \mathring{H}^1(\Omega(h); \Gamma_u)^4$ as $h \to +0$, we have to assume an additional smoothness of the matrix A, for exemple, in the ball $\mathbb{B}_R = \{x : |x| < R\}$ the inclusion

$$A \in C^{2,\alpha}(\overline{\mathbb{B}}_R)^{9\times 9} \tag{30}$$

is valid, where $C^{k,\alpha}(\Xi)$ is the Hölder space with the standard norm

$$\|v; C^{k,\alpha}(\Xi)\| = \sum_{j=1}^{k} \sup_{x\in\Xi} |\nabla_x^j v(x)| + \sup_{x,y\in\Xi} |x-y|^{-\alpha} |\nabla_x^k v(x) - \nabla_y^k v(y)|$$

and $\nabla_x^k v$ denotes the family of all derivatives of v of order k. Since the matrix differential operator

$$L(x,\nabla_x) = D(-\nabla_x)^\top A(x) D(\nabla_x) \tag{31}$$

is elliptic (see Section 3.3 below), a solution $u \in H^1(\mathbb{B}_R)^4$ of the system (9) in $\mathbb{B}_R$ with the right-hand side

$$f \in C^{0,\alpha}(\mathbb{B}_R)^4,\ \alpha \in (1/2, 1), \tag{32}$$

falls into the space $C^{2,\alpha}(\mathbb{B}_{R'})^4$ for any $R' \in (0, R)$. This fact is due to local estimates of solutions to elliptic systems [1]. Note that (32) provides the estimate

$$|f(x) - f(0)| \le c|x|^\alpha,\ x \in \mathbb{B}_R. \tag{33}$$

We also need the Taylor formula

$$|u(x) - d(x)a - D(x)^\top \varepsilon^0 - U(x)| \le c|x|^{2+\alpha},\ x \in \mathbb{B}_{R'}, \tag{34}$$

where $D(x)^\top$ is the matrix in (5) under the substitution $\nabla_x \mapsto x$,

$$\varepsilon^0 = D(\nabla_x)u(0) \in \mathbb{R}^9, \tag{35}$$

$d(x)a$ with $a \in \mathbb{R}^7$ implies a rigid motion in the mechanical component and a constant potential in the electric one,

(36)
$$d(x) = \begin{pmatrix} d^{\mathsf{M}}(x) & 0 \\ \mathbf{0} & \mathbf{0} & 1 \end{pmatrix},\ d^{\mathsf{M}}(x) = \begin{pmatrix} 1 & 0 & 0 & 0 & -2^{-1/2}x_3 & 2^{-1/2}x_2 \\ 0 & 1 & 0 & 2^{-1/2}x_3 & 0 & -2^{-1/2}x_1 \\ 0 & 0 & 1 & -2^{-1/2}x_2 & 2^{-1/2}x_1 & 0 \end{pmatrix}.$$

We emphasize a similarity of the matrices $D^{\mathsf{M}}(x)^\top$ and $d^{\mathsf{M}}(x)$. Finally, U in (34) is a quadratic term, i.e.,

$$U(tx) = t^2 U(x),\ t > 0,\ x \in \mathbb{R}^3. \tag{37}$$

Remark 3.1. *The factor* $\sqrt{2}$ *is present in the strain column* (3) *in order to equalize the natural norms for tensors of rank* 2 *with the norms of corresponding columns of height* 6*. As a result, an orthogonal transformation of the Cartesian coordinate system x implies the orthogonal transformations for all columns introduced to replace tensors (see, e.g.,* [29, Ch.2]*). By the factor* $2^{-1/2}$ *in* (36)*, we also achieve the relations*

$$\begin{aligned} &D(\nabla_x)D(x)^\top = \mathbb{I}_{9\times 9},\ D(\nabla_x)d(x) = \mathbb{O}_{9\times 7}, \\ &d(\nabla_x)^\top d(x)|_{x=0} = \mathbb{I}_{7\times 7},\ d(\nabla_x)^\top D(x)^\top|_{d=0} = \mathbb{O}_{7\times 9}, \end{aligned} \tag{38}$$

where $\mathbb{I}_{n\times n}$ *and* $\mathbb{O}_{m\times n}$ *stand for the unit and null matrices of size* $n \times n$ *and* $m \times n$*, respectively. Notice that* (35) *follows from the first couple of the relations* (38) *and our way to write the Taylor formula.*

By (30), we particularly obtain

$$A(x) = A^0 + \sum_{j=1}^{3} x_j A^j + \widetilde{A}(x),\ |\widetilde{A}_{pq}(x)| \le c|x|^2,\ x \in \mathbb{B}_R, \tag{39}$$

with the constant (9×9)-matrices A^j so that matrix (31) of differential operator gets the decomposition

$$L(x, \nabla_x) = L^0(\nabla_x) + L'(x, \nabla_x) + \widetilde{L}(x, \nabla_x). \tag{40}$$

Inserting the Taylor formula for u into the equation (9) and using (39) yield

$$L^0(\nabla_x)U(x) - \sum_{j=1}^{3} D(e_j)^\top A^j \varepsilon^0 = f(0). \tag{41}$$

Here $e_j = (\delta_{j,1}, \delta_{j,2}, \delta_{j,3})^\top$. Since U is quadratic in x (see (37)), the first term on the left hand-side is independent of x.

Remark 3.2. *To guarantee formulae* (33) *and* (34) *with* $\alpha \in (0, 1/2)$, *we could assume* $f \in H^2(\mathbb{B}_R)^4$ *while deriving* $u \in H^4(\mathbb{B}_{R'})^4$ *from local estimates for solutions of elliptic systems (see* [1]*). This is due to the Sobolev embedding theorem* $H^{l+2} \subset C^{l,\alpha}$ *in* $\mathbb{R}^3$ *for any* $\alpha \in (0, 1/2)$*. However, in Theorem 4.1 and Remark 4.2 we shall see that we really need* $\alpha > 1/2$*. The latter requires, for example,* $f \in H^3(\mathbb{B}_R)^4$*, and, therefore, we prefer here to use the Hölder scale.*

3.2. **The asymptotic ansatz.** Based on general results in [25], we accept the following asymptotic ansatz for the solution u^h of the singularly perturbed problem (25)-(28) :

$$u^h(x) = u(x) + \chi(x)(hw^1(\xi) + h^2 w^2(\xi)) + h^3 \mathbf{u}(x) + \dots \tag{42}$$

Here u is a solution of the limit problem (9)-(11), w^1 and w^2 are terms of the boundary layer type, and $\mathbf{u}$ is the main regular corrector. The cut-off function $\chi \in C_c^\infty(\Omega)$ is equal to one in the ball $\mathbb{B}_{R/3}$ and null outside $\mathbb{B}_{2R/3}$ so that, now, we fix $h_0 > 0$ such that $\omega_h \subset \mathbb{B}_{R/3}$ for $h \in (0, h_0]$.

In view of (24), the coordinate dilation $x \mapsto \xi = h^{-1}x$ removes the boundary $\partial\Omega$ close to infinity and the formal limit passage $h \to +0$ makes the exterior domain $\Xi = \mathbb{R}^3 \setminus \overline{\omega}$ from the nucleated domain $\Omega(h)$. Moreover, the decomposition (40) yields

$$L(x, \nabla_x) = L(h\xi, h^{-1}\nabla_\xi) = h^{-2}L^0(\nabla_\xi) + h^{-1}L'(\xi, \nabla_\xi) + \dots \tag{43}$$

Similarly, for the Neumann boundary operator $N^h(x, \nabla_x)$ on the left hand-side of (27), we have

$$N^h(x, \nabla_x) = h^{-1}N^0(\xi, \nabla_\xi) + h^0 N'(\xi, \nabla_\xi) + \dots \tag{44}$$

where

$$N^0(\xi, \nabla_\xi) = D(n^\omega(\xi))^\top A^0 D(\nabla_x),\ N'(\xi, \nabla_\xi) = D(n^\omega(\xi))^\top \sum_{j=1}^{3} \xi_j A^j D(\nabla_\xi), \tag{45}$$

and n^ω is the unit vector of the outward normal on $\partial\omega$.

Let us derive the exterior boundary value problems for w^1 and w^2. First, we insert the ansatz (42) into (25), make use of the expansion (44), and collect coefficients written in the fast variables ξ for similar powers of the small parameter h. As a result, we obtain systems of differential equations in Ξ for w^1 and w^2 (see (46) and (47) below). Second, we calculate the discrepancy left by the leading asymptotic term $u(x)$ in the boundary conditions (27). Namely, by means of (34), (44), we derive that

$$N^h(x,\nabla_x)u(x) = D(n^\omega(\xi))^\top \left(A^0 + h\sum_{j=1}^{3} \xi_j A^j \right) \varepsilon^0 + hN^0(\xi,\nabla_\xi)U(\xi) + \dots$$

Finally, we write the problems

$$\begin{aligned} &L^0(\nabla_\xi)w^1(\xi) = 0,\ \xi\in\Xi,\\ &N^0(\xi,\nabla_\xi)w^1(\xi) = -D(n^\omega(\xi))^\top A^0\varepsilon^0,\ \xi\in\partial\omega, \end{aligned} \tag{46}$$

and

(47)

$$\begin{aligned} &L^0(\nabla_\xi)w^2(\xi) = -L'(\xi,\nabla_\xi)w^1(\xi),\ \xi\in\Xi,\\ &N^0(\xi,\nabla_\xi)w^2(\xi) = -N'(\xi,\nabla_\xi)w^1(\xi) - N'(\xi,\nabla_\xi)D(\xi)^\top\varepsilon_0 - N^0(\xi,\nabla_\xi)U(\xi),\ \xi\in\partial\omega. \end{aligned}$$

3.3. **The exterior problem in piezoelectricity.** The polynomial property [30, 31] of a formally self-adjoint system of differential equations delivers plenty of results for the exterior boundary value problem in Ξ such as the ellipticity, the solvability, asymptotic expansions of solutions, and intrinsic integral characteristics, i.e. the polarization matrices (see [35, Ch.6], [31, 33] and [36] in shape optimization). As it has been mentioned, the piezoelectricity system (9) is not formally self-adjoint, however, introducing the imaginary potential iu_4^{E} (see [31, Example 1.13]) and the column $u_{(i)} = (u_1^{\mathsf{M}}, u_2^{\mathsf{M}}, u_3^{\mathsf{M}}, iu_4^{\mathsf{E}})^\top$ brings the sesquilinear form

$$q_{(i)}(u_{(i)}, v_{(i)}; \Xi) = (A^0_{(i)} D(\nabla_\xi)u_{(i)}, D(\nabla_\xi)v_{(i)})_\Xi \tag{48}$$

where i is the imaginary unit and $A^0_{(i)}$ stands for modified matrix (23),

$$A^0_{(i)} = \begin{pmatrix} A^{0\mathsf{MM}}, & iA^{0\mathsf{ME}} \\ iA^{0\mathsf{EM}}, & A^{0\mathsf{EE}} \end{pmatrix} = A^0_{(Re)} + iA^0_{(Im)}, \tag{49}$$

while both $A^0_{(Re)}$ and $A^0_{(Im)}$ are real symmetric and $A^0_{(Re)}$ is positive definite. The sesquilinear form (48) is not Hermitian in the case $A^{0\mathsf{ME}} \neq \mathbb{O}_{6\times 3}$, but it enjoys the polynomial property [30, 32, 31]:

$$q_{(i)}(u_{(i)}, u_{(i)}; \Upsilon) = 0 \iff u_{(i)} \in \mathcal{P}|_\Upsilon, \tag{50}$$

where Υ is any domain in $\mathbb{R}^3$ and $\mathcal{P} = \{p : p(x) = d(x)a,\ a\in\mathbb{C}^7\}$ is a polynomial subspace of dimension 7 generated by the matrix in (36).

The above observations made in [32, 31] and the investigation scheme [35, Ch.6] provide all results we formulate below with exception for the polarization matrix and here the most attention is paid to this integral characteristics of the opening $\overline{\omega}$ in the homogeneous piezoelectric space.

Let $V_0^1(\Xi)$ be the Kondratiev space [18] obtained by the completion of the linear space $C_c^\infty(\overline{\Xi})$ (infinitely differentiable functions with compact supports) with respect to the Dirichlet integral norm $\|\nabla_\xi w; L^2(\Xi)\|$. Applying the one-dimensional Hardy inequality in the radial variable $\rho = |\xi|$, we use the equivalent norm

$$\|w; V_0^1(\Xi)\| = (\|\nabla_\xi w; L^2(\Xi)\|^2 + \|\rho^{-1} w; L^2(\Xi)\|^2)^{1/2}. \tag{51}$$

The problem (46) with the right-hand side $g \in L^2(\partial\omega)^4$ in the Neumann boundary conditions can be reformulated as the integral identity, similarly to (12)

$$(A^0 D(\nabla_\xi)w, D(\nabla_\xi)v)_\Xi = (g, v)_{\partial\omega}, \ v \in V_0^1(\Xi)^4. \tag{52}$$

Proposition 3.1. *For any $g \in L^2(\partial\omega)^4$, the problem* (52) *has a unique solution $w \in V_0^1(\Xi)^4$ and the estimate $\|w; V_0^1(\Xi)\| \le c\|g; L^2(\partial\omega)\|$ is valid.*

Although $\partial\omega$ and g are not smooth, the solution w in Proposition 3.1 is infinitely differentiable outside of any neighborhood $\mathcal{V}$ of the set $\overline{\omega}$ (recall the local estimates in [1] mentioned above). To describe the behavior of $w(\xi)$ as $\rho \to \infty$, we introduce the fundamental matrix $\Phi(x)$ of size 4×4 for the operator $L^0(\nabla_\xi)$ in $\mathbb{R}^3$ (see [10, 12]). This matrix is positive homogeneous of degree -1, namely,

$$\Phi(t\xi) = t^{-1}\Phi(\xi), \ t > 0, \ \xi \in \mathbb{R}^3 \setminus \{0\}. \tag{53}$$

The next assertion is due to [18], [27] (see also [43] and, e.g., [35, Ch.6]).

Proposition 3.2. *The solution $w \in V_0^1(\Xi)^4$ of the problem* (52) *admits the asymptotic form*

$$w(\xi) = (d(-\nabla_\xi)^\top \Phi(\xi)^\top)^\top a + (D(-\nabla_\xi)\Phi(\xi)^\top)^\top b + \widetilde{w}(\xi), \tag{54}$$

$$|\nabla_\xi^k \widetilde{w}(\xi)| \le c_k \rho^{-3-k}, \ k \in \mathbb{N}_0 = \{0, 1, 2, \dots\}, \ \xi \in \mathbb{R}^3 \setminus \mathcal{V}, \tag{55}$$

where $a \in \mathbb{R}^7$ and $b \in \mathbb{R}^9$ while $|a| + |b| \le c\|g; L^2(\partial\omega)\|$.

Remark 3.3. *Formula* (54) *contains the matrices d and D in* (36) *and* (5). *Let $d^1(\xi), \dots, d^7(\xi)$ be columns of $d(\xi)$ and let $D_1(\xi), \dots, D_9(\xi)$ be strings of $D(\xi)$. Then we rewrite* (54) *in the form of strings*

$$w(\xi)^\top = \sum_{j=1}^{7} a_j d^j(-\nabla_\xi)^\top \Phi(\xi)^\top + \sum_{k=1}^{9} B_k D_k(-\nabla_\xi)\Phi(\xi)^\top + \widetilde{w}(\xi)^\top.$$

Therefore, the asymptotic terms detached in (54) *are but a linear combination of columns of the fundamental matrix $\Phi(\xi)$ (with the coefficients a_1, a_2, a_3 and a_7; cf.*(36)*) and of the first-order derivatives of the columns (with the coefficients a_4, a_5, a_6 and $b_1, \dots, b_9$).*

The columns $d^1, \dots, d^7$ satisfy the homogeneous problem (46). However, the columns are not in the weighted space $V_0^1(\Xi)^4$ by the lack of their decay rate and, hence, $d^j(\xi)$ are not solutions of the homogeneous ($g = 0$) problem (52) in Proposition 3.2. According to the general method [26] such solutions are used to compute the coefficients in the asymptotic expansion (54). We are going to use this method twice. First, we observe that the right-hand side g in (46) verifies the orthogonality conditions

$$\int_{\partial\omega} d(\xi)^\top g(\xi) ds_\xi = 0 \in \mathbb{R}^7. \tag{56}$$

Indeed, by (38), we get

(57)
$$\left(\int\limits_{\partial\omega} d(\xi)^\top g(\xi) ds_\xi\right)^\top = -(A^0\varepsilon^0)^\top \int\limits_{\partial\omega} D(n^\omega(\xi)) d(\xi) ds_\xi = -(A^0\varepsilon^0)^\top \int\limits_{\omega} D(\nabla_\xi) d(\xi) d\xi = 0.$$

Proposition 3.3. *Under orthogonality condition* (56)*, the column $a \in \mathbb{R}^7$ in* (54) *vanishes.*

The proof is commented in Remark 3.6.

Let $W^j \in V_0^1(\xi)^4$ be a solution to the problem (52) with the specific right-hand side

$$g^j(\xi) = -D(n^\omega(\xi))^\top A^0 \mathbf{e}_j; \tag{58}$$

here $j = 1, \ldots, 9$, $\mathbf{e}_j = (\delta_{j,1}, \ldots, \delta_{j,9})^\top$ is the unit column in $\mathbb{R}^9$, and $\delta_{j,k}$ stands for the Kronecker symbol. Recalling the problem (46) for the boundary layer term w^1, we see that

$$w^1(\xi) = W(\xi)\varepsilon^0 \tag{59}$$

with the (4×9)-matrix function W composed from the columns $W^1, \ldots, W^9$ of height 4,

$$W = (W^1, \ldots, W^9). \tag{60}$$

By Proposition 3.3 and the relation (57), we conclude the expansions

$$W^j(\xi)^\top = \sum_{p=1}^{9} M_{jp} D_p(\nabla_\xi)\Phi(\xi)^\top + \widetilde{W}^j(\xi)^\top \tag{61}$$

where the remainders $\widetilde{W}^j(\xi)$ obey the estimates (55). The coefficients M_{jp} in (61) form the matrix of size 9×9

$$M = M(A^0, \omega) \tag{62}$$

which, in the analogy with [49, 34, 40] and others, is called *the polarization matrix* of the opening ω in the homogeneous piezoelectric space.

As in Section 2.3, our study of general properties of (62) relies on both formulations (12) and (22) of the piezoelectricity problem. Hence, we have to perform the same sign changes as in (23),

$$M = \begin{pmatrix} M^{\mathsf{MM}} & M^{\mathsf{ME}} \\ M^{\mathsf{EM}} & M^{\mathsf{EE}} \end{pmatrix} \mapsto M_{(=)} = \begin{pmatrix} M^{\mathsf{MM}} & -M^{\mathsf{ME}} \\ M^{\mathsf{EM}} & -M^{\mathsf{EE}} \end{pmatrix}. \tag{63}$$

Theorem 3.4. *Entries of the modified polarization matrix $M_{(=)}$ satisfy the relation*

$$(M_{(=)})_{jp} = -Q^0_{(-)}(W^j, W^p; \Xi) - (A^0_{(-)})_{jp} mes_3\omega, \;\; j, p = 1, \ldots, 9, \tag{64}$$

where $Q^0_{(-)}$ is the quadratic form in (22) *with the matrix $A^0_{(-)} = A_{(-)}(0)$ (see* (23) *and* (39)*).*

Proof. By (58) and (38), the sum $\mathcal{W}^j(\xi) = D_j(\xi)^\top + W^j(\xi)$ verifies the homogeneous problem (46). In the method [26] these solutions play the same role as it was registered for the columns $d^1, \ldots, d^7$ above Proposition 3.3. We underline that the vector function

$$\mathcal{W}^j_{(-)} = (\mathcal{W}^{j\mathsf{M}}_1, \mathcal{W}^{j\mathsf{M}}_2, \mathcal{W}^{j\mathsf{M}}_3, -\mathcal{W}^{j\mathsf{E}})^\top \tag{65}$$

verifies a homogeneous boundary value problem which is formally adjoint for (46) and involves the differential operators $L^0_{(\top)}$ and $N^0_{(\top)}$ constructed from L^0 and N^0 in (40) and (45), respectively, by replacing A^0 with the transposed matrix $(A^0)^\top$. Clearly, $L^0_{(\top)}(\nabla_\xi) = L^0(\nabla_\xi)^*$ is the formally adjoint for the differential operator $L^0(\nabla_\xi)$.

We insert W^j and $\mathcal{W}^p_{(-)}$ into the Green formula written for the truncated domain $\Xi_R = \Xi \cap \mathbb{B}_R$ and choose the radius of the ball $\mathbb{B}_R = \{\xi : |\xi| < R\}$ such that the sphere $\mathbb{S}_R = \partial\mathbb{B}_R$ envelopes the set $\overline{\omega}$. We have

$$(L^0 W^j, \mathcal{W}^p_{(-)})_{\Xi_R} + (N^0 W^j, \mathcal{W}^p_{(-)})_{\partial\omega\cup\mathbb{S}_R} = (W^j, L^0_{(\top)}\mathcal{W}^p_{(-)})_{\Xi_R} + (W^j, N^0_{(\top)}\mathcal{W}^p_{(-)})_{\partial\omega\cup\mathbb{S}_R}. \tag{66}$$

Since $L^0\mathcal{W}^j = 0$ provides $L^0_{(\top)}\mathcal{W}^j_{(-)} = 0$, the integrals over Ξ_R in (66) vanish. Furthermore, $N^0_{(\top)}(\xi, \nabla_\xi)\mathcal{W}^p_{(-)}(\xi) = 0$, $\xi \in \partial\omega$. Thus, (66) converts into

$$(N^0 W^j, \mathcal{W}^p_{(-)})_{\partial\omega} = (W^j, N^0_{(\top)}\mathcal{W}^p_{(-)})_{\mathbb{S}_R} - (N^0 W^j, \mathcal{W}^p_{(-)})_{\mathbb{S}_R} \tag{67}$$

where $N^0(\xi, \nabla_\xi) = D(|\xi|^{-1}\xi)^\top A^0 D(\xi)$ on the sphere $\mathbb{S}_R$.

Taking into account the estimates (55) for $\widetilde{W}^j$ and the concomitant estimates $|\nabla^k_\xi W^p(\xi)| \le c_p \rho^{-1-k}$, we obtain that the right-hand side I^{jp}_{right} of (66) satisfies

$$I^{jp}_{right} = (\Sigma^j, N^0_{(\top)} D^\top_{p(-)})_{\mathbb{S}_R} + O(R^{-1})$$

where Σ^j means the asymptotic term detached in (61) and $D_{p(-)}(\xi)^\top$ is a column of the matrix $D(\xi)^\top$ transformed according to (58). Understanding integrals over the ball $\mathbb{B}_R$ in the framework of the theory of distributions, we obtain

$$\begin{aligned} I^{jp}_{right} &= (L^0\Sigma^j, D^\top_{p(-)})_{\mathbb{B}_R} - (\Sigma^j, L^0_{(\top)} D^\top_{p(-)})_{\mathbb{B}_R} + O(R^{-1}) \\ &= \sum_{q=1}^{9} M_{jq} \int_{\mathbb{B}_R} D_{p(-)}(\xi) D_q(\nabla_\xi)^\top \delta(\xi) d\xi + O(R^{-1}) \\ &= \sum_{q=1}^{9} M_{jq} D_q(-\nabla_\xi) D_{p(-)}(\xi)^\top|_{\xi=0} + O(R^{-1}) \\ &= \left\{ \begin{array}{lll} -M_{jp} & \text{for} & p = 1, \ldots, 6, \\ M_{jp} & \text{for} & p = 7, 8, 9 \end{array} \right\} + O(R^{-1}) = -(M_{(=)})_{jp} + O(R^{-1}). \end{aligned} \tag{68}$$

Here we have used that, first, $D_{p(-)}(\xi)$ is linear in ξ and, therefore, $L^0_{(\top)}D^\top_{p(-)} = 0$ and, second,

$$L^0(\nabla_\xi)\Sigma^j(\xi) := \sum_{q=1}^{9} M_{jq}L^0(\nabla_\xi)(D_q(-\nabla_\xi)\Phi(\xi)^\top)^\top = \sum_{q=1}^{9} M_{jq}D_q(-\nabla_\xi)^\top\delta(\xi)$$

caused by the formula $L^0(\nabla_\xi)\Phi(\xi) = \delta(\xi)\mathbb{I}_{4\times 4}$, i.e., by the definition of the fundamental matrix Φ.

Let us process the left-hand side I^{jp}_{right} of (66). Again integrating by parts, this time in the domains Ξ and ω, it follows that

$$\begin{aligned} I^{jp}_{left} &= (N^0W^j, W^p_{(-)})_{\partial\Xi} - (N^0D^\top_j, D^\top_{p(-)})_{\partial\omega} \\ &= Q^0(W^j, W^p_{(-)}; \Xi) + Q^0(D^\top_j, D^\top_{p(-)}; \omega) \\ &= Q^0_{(-)}(W^j, W^p; \Xi) + (A^0_{(-)})_{jp} mes_3\omega, \end{aligned} \tag{69}$$

where $mes_3\omega$ is the volume of ω. Note that, first, the equality $N^0W^j = -N^0D^\top_j$ on $\partial\omega$ is inherited from (58) and (38), second, n^ω and $-n^\omega$ imply the outward normals with respect to the sets Ξ and ω, respectively, and, third,

$$\begin{aligned} Q^0(u, v_{(-)}; \Xi) &= (A^0D(\nabla_\xi)u, D(\nabla_\xi)v_{(-)})_\Xi \\ &= (A^0_{(-)}D(\nabla_\xi)u, D(\nabla_\xi)v)_\Xi = Q^0_{(-)}(u, v; \Xi), \\ Q^0_{(-)}(D^\top_j, D^\top_p; \omega) &= (A^0_{(-)}\mathbf{e}_j, \mathbf{e}_p)_\omega = (A^0_{(-)})_{jp} mes_3\omega. \end{aligned} \tag{70}$$

Comparing (68) and (69), we send R to $+\infty$ and obtain the desired relation (64).■

Theorem 3.4 ensures the matrix $M_{(=)}$ in (63) to be symmetric, in particular, $M^{\mathsf{ME}} = -(M^{\mathsf{EM}})^\top$. However, in contrast to the polarization matrix in elasticity (cf. [49, 34, 40]) neither $M_{(=)}$, nor M enjoy the positivity/negativity property. In the case $A^{\mathsf{ME}} = \mathbb{O}_{6\times 3}$ the piezoelectricity problem decouples into the elasticity and electricity problems so that,

$$M^{\mathsf{MM}} < 0,\ M^{\mathsf{EE}} > 0,\ M^{\mathsf{ME}} = -(M^{\mathsf{EM}})^\top = \mathbb{O}_{6\times 3}, \tag{71}$$

provided, e.g., $mes_3\omega > 0$. We emphasize that in (71) M^{EE} is but the virtual mass tensor (see [44]). By the perturbation argument, the matrix M has six negative and three positive eigenvalues, if the matrix A^{ME} is sufficiently small (cf. Section 4.4). However, for arbitrary A^{ME}, this property is still an open question.

We have examined the first asymptotic term (59) of the boundary layer type in the asymptotic ansatz (42). By the representation (61) (see Remark 3.3), we write the expansion of $w^1(\xi)$ for $\xi \to +\infty$ in the matrix form as follows

$$w^1(\xi) = (D(\nabla_x)\Phi(\xi)^\top)^\top M^\top\varepsilon^0 + \widetilde{w}^1(\xi). \tag{72}$$

The remainder $\widetilde{w}^1$ obeys the estimates (55).

Remark 3.5. *Formula* (72) *can be derived in the following way:*

$$
\begin{aligned}
W^j(\xi) &= \sum_{p=1}^{9} M_{jp} \sum_{q=1}^{3} \frac{\partial \Phi}{\partial \xi_q}(\xi) D_p(e_q)^\top + \widetilde{W}^j(\xi) \\
&= \sum_{p=1}^{9} M_{jp} \left(\sum_{q=1}^{3} D_p(e_q) \frac{\partial \Phi}{\partial \xi_q}(\xi)^\top \right)^\top + \widetilde{W}^j(\xi) \\
&= \left(\sum_{p=1}^{9} M_{jp} D_p(\nabla_\xi)\Phi(\xi)^\top \right)^\top + \widetilde{W}^j(\xi)
\end{aligned}
$$

where $M_1, \dots, M_9$ are strings of the matrix M.

3.4. **The second term in the boundary layer.** By virtue of (39) and (40), the operator

$$L'(\xi, \nabla_\xi) = D(-\nabla_\xi)^\top \left(\sum_{j=1}^{3} \xi_j A^j D(\nabla_\xi) \right) \tag{73}$$

gets the following homogeneity property:

$$L'(\xi, \nabla_\xi)\rho^\lambda \varphi(\theta) = \rho^{\lambda-1}\psi(\theta),\ \xi \in \mathbb{R}^3 \setminus \{0\}. \tag{74}$$

Here $\lambda \in \mathbb{R}$, (ρ, θ) are the spherical coordinates in $\mathbb{R}^3$, $\rho = |\xi|$ and $\theta = \rho^{-1}\xi \in \mathbb{S}_1$, and $\varphi, \psi \in C^\infty(\mathbb{S}_1)^4$. Thus, by means of (59) and (61), (55), (53), we obtain that

$$F'(\xi) = -L'(\xi, \nabla_\xi)w^1(\xi) = D(\nabla_\xi)^\top(\rho^{-2}\Psi(\xi)) + O(\rho^{-2}),\ \rho \to +\infty, \tag{75}$$

while the formula can be differentiated under the standard convention $\nabla_x O(\rho^{-\lambda}) = O(\rho^{-\lambda-1})$. Due to the definition (51) of the Kondratiev norm the right-hand side of (75) gives rise to the continuous functional

$$V_0^1(\Xi)^4 \ni v \mapsto (F', v)_\Xi,$$

$$|(F', v)_\Xi| \le c \int_\Xi \rho^{-3}|v(\xi)| d\xi \le c \left(\int_\Xi \rho^{-4} d\xi \right)^{1/2} \|\rho^{-1}v; L^2(\Xi)\| \le C\|v; V_0^1(\Xi)\|.$$

Thus, similarly to Proposition 3.1, we obtain the existence of a unique solution $w^2 \in V_0^1(\Xi)^4$ to the problem (47). Now, we need to examine the behavior of $w^2(\xi)$ as $\rho \to +\infty$. According to [18] (see also [35, §3.5]), first of all, we have to determine the power-law solution

$$Z(\xi) = \rho^{-1}\mathcal{Z}(\theta) \tag{76}$$

to the system of differential equations

$$L^0(\nabla_\xi)Z(\xi) = \rho^{-3}\mathcal{F}(\theta) := D(\nabla_x)^\top(\rho^{-2}\Psi(\theta)),\ \xi \in \mathbb{R}^3 \setminus \{0\}, \tag{77}$$

with the right-hand side taken from (75). Note that, in general, the multiplier $\mathcal{W}$ in (76) may be linear in $\ln \rho$ but, owing to a special form of $\mathcal{T}$, the next lemma proves the absence of the logarithm.

Lemma 3.1. *The system* (77) *admits the power-law solution of form* (76)*, whose angular part* $\mathcal{W}(\theta)$ *is defined up to the linear combination* $c_1\Phi^1(\theta)+\cdots+c_4\Phi^4(\theta)$*, where* $c_j\in\mathbb{R}$ *and* $\Phi^j(\theta)$ *is the trace on the unit sphere* $\mathbb{S}_1$ *of the column* $\Phi^j(\xi)$ *in the fundamental matrix* Φ*.*

Proof. After separation of variables and rewriting the operator $L^0(\nabla_\xi)=\rho^{-2}\mathfrak{L}(\theta,\nabla_\theta,\rho\partial_\rho)$ in the spherical coordinates (ρ,θ), the system (77) takes the form

$$\mathfrak{L}(\theta,\nabla_\theta,-1)\mathcal{Z}(\theta)=\mathcal{F}(\theta),\ \theta\in\mathbb{S}_1. \tag{78}$$

By the Fredholm alternative, this system on the unit sphere has a solution if and only if the right-hand side $\mathcal{F}$ is orthogonal to all solutions of the formally adjoint homogeneous system. Owing to [26] (see also [35, Lemma 3.5.9]), the formally adjoint operator for $\mathfrak{L}(\theta,\nabla_\theta,-1)$ is nothing but $\mathfrak{L}_{(\top)}(\theta,\nabla_\theta,0)$, where

$$\rho^{-2}\mathfrak{L}_{(\top)}(\theta,\nabla_\theta,\rho\partial_\rho)=L^0_{(\top)}(\nabla_\xi)=L^0(\nabla_\xi)^*. \tag{79}$$

By virtue of the polynomial property (50), any power-law solution $X(\xi)=\rho^0\mathcal{X}(\xi)$ of $L^0_{(\top)}(\nabla_\xi)X=0$ in $\mathbb{R}^3\setminus\{0\}$ is a constant column in $\mathbb{R}^4$. Thus, it suffices to verify the orthogonality condition

$$\int_{\mathbb{S}_1}\mathcal{F}(\theta)ds_\theta=0\in\mathbb{R}^4. \tag{80}$$

Let $R>r>0$ and let Θ be the annulus $\{\xi:r<\rho<R\}$. We have

$$\ln\Big(\frac{R}{r}\Big)\int_{\mathbb{S}_1}\mathcal{F}(\theta)ds_\theta=\int_r^R\rho^{-1}d\rho\int_{\mathbb{S}_1}\mathcal{F}(\theta)ds_\theta=\int_\Theta\rho^{-3}\mathcal{F}(\theta)d\xi$$
$$=\int_\Theta D(\nabla_\xi)^\top(\rho^{-2}\psi(\theta))d\xi=\int_{\mathbb{S}_R}D(\rho^{-1}\xi)^\top(\rho^{-2}\Psi(\theta))ds_\xi-\int_{\mathbb{S}_r}D(\rho^{-1}\xi)^\top(\rho^{-2}\Psi(\theta))ds_\xi=0.$$

We have used here the Gauss formula and the fact that the integrands at $\rho=R$ and $\rho=r$ are equal to $R^{-2}D(\theta)^\top\Psi(\theta)$ and $r^{-2}D(\theta)^\top\Psi(\theta)$, respectively, so that the integrals cancel each other.

Thus, the compatibility condition (80) holds true and the system (78) admits a solution. It remains to recall that any power-law solution (76) of the homogeneous system (77) becomes a linear combination of the fundamental matrix columns.■

To assure the uniqueness of the solution (76), we impose the condition

$$\int_{\mathbb{S}_1}D(\theta)^\top A^0\mathfrak{D}(\theta,\nabla_\theta,-1)\mathcal{Z}(\theta)ds_\theta=0\in\mathbb{R}^4, \tag{81}$$

where $\rho^{-1}\mathfrak{D}(\theta,\nabla_\theta,\rho\partial_\rho)$ is the matrix operator $D(\nabla_x)$ written, similarly to (79), in the spherical coordinates (ρ,θ).

Now, we are in position to write an expansion at infinity for the second boundary layer term in (42).

Proposition 3.4. *The solution $w^2 \in V_0^1(\Xi)^4$ of the problem* (47) *admits the asymptotic form*

$$w^2(\xi) = Z(\xi) + \Phi(\xi)C + \widetilde{w}^2(\xi), \tag{82}$$

$$|\nabla_\xi^k \widetilde{w}^2(\xi)| \leq c_{k,\beta}\rho^{-2-k+\beta}, \ k \in \mathbb{N}_0, \ \xi \in \mathbb{R}^3 \setminus \mathcal{V}, \tag{83}$$

where $\beta > 0$ is arbitrary, Z is a power-law solution of form (76) *and $C \in \mathbb{R}^4$ is determined as follows:*

$$C = -f(0)mes_3\omega + J \in \mathbb{R}^4, \tag{84}$$

$$J = \int\limits_{\mathbb{S}_1} D(\theta)^\top \sum_{j=1}^{3} \xi_j A^j D(\nabla_\xi)(D(\nabla_\xi)\Phi(\xi)^\top)^\top ds_\xi M^\top \varepsilon^0. \tag{85}$$

Proof. The asymptotic expansion (82) with a certain column C and the estimates (83) result from [18] and [27], respectively (see also [35, Ch.3]). We again employ the method proposed in [26] to evaluate the constant column C. Now, we use the Green formula in Ξ_R for w^2 and $\mathsf{e_p} = (\delta_{\mathsf{p},1}, \dots, \delta_{\mathsf{p},4})^\top$. Recalling (47), we have

(86)
$$I_{left} := -\int\limits_{\Xi_R} \mathsf{e}_p^\top L' w^1 d\xi - \int\limits_{\partial\omega} \mathsf{e}_p^\top N' w^1 ds\xi - \int\limits_{\partial\omega} \mathsf{e}_p^\top N' D(\xi)\varepsilon^0 ds_\xi - \int\limits_{\partial\omega} \mathsf{e}_p^\top N' U ds_\xi$$
$$= \int\limits_{\Xi_R} \mathsf{e}_p^\top L^0 w^2 d\xi + \int\limits_{\partial\omega} \mathsf{e}_p^\top N^0 w^2 ds\xi = \int\limits_{\mathbb{S}_R} \mathsf{e}_p^\top N^0 w^2 ds\xi =: I_{right}.$$

Here $N^0(\xi, \nabla_\xi) = D(\theta)^\top A^0 D(\nabla_\xi)$ on the sphere $\mathbb{S}_R$ with the unit normal vector $\theta = \rho^{-1}\xi$ (cf. (45) and (81)). Similarly to the calculation (68), using (82) and (81), we get

$$\begin{aligned} I_{right} &= -\int\limits_{\mathbb{S}_R} \mathsf{e}_p^\top N^0 \mathcal{Z} ds_\xi - \int\limits_{\mathbb{S}_R} \mathsf{e}_p^\top N^0 \Phi ds_\xi C + O(R^{-1}) = \\ &= \int\limits_{\mathbb{B}_R} \mathsf{e}_p^\top L^0 \Phi d\xi C + O(R^{-1}) = C_p + O(R^{-1}). \end{aligned} \tag{87}$$

By integrating by parts, the last couple of integrals in I_{left} turns into

(88)
$$-\int\limits_{\Xi_R} \mathsf{e}_p^\top L' w^1 d\xi - \int\limits_{\partial\omega} \mathsf{e}_p^\top N' w^1 ds\xi = \int\limits_{\mathbb{S}_R} \mathsf{e}_p^\top D(\theta)^\top \sum_{j=1}^{3} \xi_j A^j D(\nabla_\xi)(D(\nabla_\xi)\Phi(\xi)^\top)^\top ds_\xi M \varepsilon^0 + O(R^{-1}).$$

Here we have applied the decomposition (72) of w^1 together with the estimate (55) for the remainder. Since its integrand is a positive homogeneous function in ξ of degree -2 (cf. (53)) the integral J_p over $\mathbb{S}_R$ in (88) is independent of the radius R and becomes an entry of column (85).

The first couple of integrals in (86) is equal to

$$\int_{\partial\omega} \mathrm{e}_p^\top N' D(\xi)\varepsilon^0 ds_\xi - \int_{\partial\omega} \mathrm{e}_p^\top N^0 U ds_\xi = -\int_{\omega} \mathrm{e}_p^\top (L' D(\xi)\varepsilon^0 + L^0 U) d\xi$$
$$= -mes_3\omega \mathrm{e}_p^\top (-\textstyle\sum_{j=1}^3 D(e_j)^\top A^j \varepsilon^0 + L^0(\nabla_\xi)U(\xi)) = -f_p(0) mes_3\omega.$$

Here, the elementary formula (41) has been taken into account.

Now the limit passage $R \to +\infty$ in (86)-(88) furnishes (84) and (85).■

Remark 3.6. *Proposition 3.3 can be proved by an application of the method* [26] *in the same way as it is made in Proposition 3.4 and Theorem 3.4. We only mention that the columns $d^1, \dots, d^7$ of the matrix $d(\xi)$ in* (36) *satisfy sumultaneously the homogeneous problem* (46) *and the formally adjoint boundary value problem in Ξ with the operators $L^0_{(\top)}(\nabla_\xi)$ and $N^0_{(\top)}(\xi, \nabla_\xi)$, respectively.*

3.5. **The regular correction term.** Let us consider now the subsequent term in the asymptotic ansatz (42), namely the regular correction term $\mathbf{u}(x)$.

By means of (72) and (82), we have

$$\begin{aligned} &hw^1(h^{-1}x) + h^2 w^2(h^{-1}x) = h(S^2(h^{-1}x) + \widetilde{w}^1(h^{-1}x)) + \\ &+ h^2(S^1(h^{-1}x) + \widetilde{w}^2(h^{-1}x)) = h^3(S^2(x) + S^1(x)) + O(h^4(|x|^{-3} + |x|^{-2})) \end{aligned} \tag{89}$$

where, according to (53) and (76), we have set

$$S^2(\xi) = (D(-\nabla_\xi)\Phi(\xi)^\top)^\top M^\top \varepsilon^0, \; S^1(\xi) = Z(\xi) + \Phi(\xi)C, \tag{90}$$
$$S^p(t\xi) = t^{-p} S^p(\xi).$$

Therefore, this is $h^3\mathbf{u}(x)$ in the asymptotic ansatz (42) that compensates the main part of a discrepancy produced by the boundary layer terms w^1 and w^2.

Taking into account the equalities $L^0 S^2 = 0$ and $L^0 S^1 = -L' S^2$ designated in two last sections, we arrive at the following representation of the discrepancy in the system (25) :

$$\begin{aligned} &\mathbf{f}(x) = -L(x,\nabla_x)(\chi(x)(S^2(x) + S^1(x))) = \\ &= -[L,\chi](S^2(x) + S^1(x)) - \chi(x)(L(x,\nabla_x) - L^0(\nabla_x) - L'(x,\nabla_x))S^2(x) - \\ &-\chi(x)(L(x,\nabla_x) - L^0(\nabla_x))S^1(x). \end{aligned} \tag{91}$$

Here $[L,\chi]$ stands for the commutator of the differential operator L and the cut-of function χ, i.e.,

$$[L,\chi] = D(-\nabla_x)^\top A(x) D(\nabla_x \chi(x)) - D(\nabla_x\chi(x))^\top A(x) D(\nabla_x). \tag{92}$$

Recalling (39) and (40), in view of (90), we obtain that

$$|\mathbf{f}(x)| \leq c|x|^{-2}. \tag{93}$$

We see that the regular correction term $\mathbf{u}$ must satisfy the piezoelectricity problem

$$D(-\nabla_x)^\top A(x) D(\nabla_x)\mathbf{u}(x) = \mathbf{f}(x), \; x \in \Omega, \tag{94}$$

$$D(n(x))^\top A(x) D(\nabla_x)\mathbf{u}(x) = 0, \; x \in \Gamma_\sigma, \; \mathbf{u}(x) = 0, \; x \in \Gamma_u. \tag{95}$$

We emphasize that the sum $h\widetilde{w}^1(h^{-1}x) + h^2\widetilde{w}^2(h^{-1}x)$ in (89) becomes of order h^4 only at a distance from the coordinate origin $x = 0$. However, we have extended equations (94) over the whole domain Ω because the singularity $O(|x|^{-2})$ of the right-hand side $\mathbf{f}(x)$ is not too strong. In particular, by (93), the functional on the right-hand side in the integral identity

$$Q(\mathbf{u}, \mathbf{v}; \Omega) = (\mathbf{f}, \mathbf{v})_\Omega, \ \mathbf{v} \in \mathring{H}^1(\Omega; \Gamma_u)^4, \tag{96}$$

serving for the problem (94), (95) (cf. (12)), is continuous due to the estimate

$$|(\mathbf{f}, \mathbf{v})_\Omega| \le c \left(\int_\Omega |x|^2 |\mathbf{f}(x)|^2 dx \right)^{1/2} \left(\int_\Omega |x|^{-2} |\mathbf{v}(x)|^2 dx \right)^{1/2} \le$$
$$\le c \left(\int_0^{diam\Omega} r^2 r^{-4} r^2 dr \right)^{1/2} \|\nabla_x \mathbf{v}; L_2(\Omega)\| \le C \|\mathbf{v}; H^1(\Omega)\|$$

and the one-dimensional Hardy inequality mentioned above (51). Hence, in the analogy with Proposition 2.1, the Lax-Milgram lemma ensures the existence and uniqueness of the solution $\mathbf{u} \in \mathring{H}^1(\Omega; \Gamma_u)^4$. These observations complete the evaluation of all asymptotic terms detached in (42).

Remark 3.7. *The singularity of* $\mathbf{f}$ *can lead to a logarithmical singularity of the solution* $\mathbf{u}$. *However, we shall need only the following inequalities with arbitrary* $\beta > 0$ *:*

$$|\mathbf{u}(x)| \le c_\beta |x|^{-\beta}, \ |\nabla_x \mathbf{u}(x)| \le c_\beta |x|^{-1-\beta} \tag{97}$$

delivered by a result in [27] *(see also* [35, §3.6]*).*

For the further usage, it is convenient to rewrite the ansatz (42) in a different form, namely

$$u^h(x) = u(x) + h^3 \mathbf{U}(x) + \chi(x)(h\widetilde{w}^1(h^{-1}x) + h^2\widetilde{w}^2(h^{-1}x)) + \widetilde{u}^h(x), \tag{98}$$

where, in accordance with (89) and (90),

$$\mathbf{U}(x) = \mathbf{u}(x) + \chi(x)(S^2(x) + S^1(x)). \tag{99}$$

In other words, we detach $hS^2(h^{-1}x)$ and $h^2S^1(h^{-1}x)$ from the boundary layer terms and attach them to the regular term $\mathbf{u}$. Therefore, the remainder $\widetilde{u}^h$ in (98) stays the same as in the original ansatz (42).

Let us derive an *almost explicit* formula for (99). To this end, let $G(x, y)$ be the Green matrix for the piezoelectricity problem (9)-(11), i.e.,

$$\begin{array}{l} D(-\nabla_x)^\top A(x) D(\nabla_x) G(x, y) = \delta(x - y) \mathbb{I}_{4\times4}, \ x \in \Omega, \\ D(n(x))^\top A(x) D(\nabla_x) G(x, y) = 0, \ x \in \Gamma_\sigma, \ u(x) = 0, \ x \in \Gamma_u \end{array} \tag{100}$$

Of course, the relations (100) are understood in the sense of distributions, so that, $G \in L^2(\Omega)^{4\times4}$, $G \in L^2(\partial\Omega)^{4\times4}$ and

$$(G, Lv)_\Omega + (G, Nv)_{\Gamma_\sigma} = v(y), \ v \in C_c^\infty(\overline{\Omega}; \Gamma_u)^4,$$

where the linear space $C_0^\infty(\overline{\Omega};\Gamma_u)$ consists of infinitely differentiable functions in $\overline{\Omega}$ which vanish on Γ_u. Since A is a smooth matrix function inside of the ball $\mathbb{B}_R$ (see (30)), the Green matrix is properly defined for $y \in \mathbb{B}_R$ (see [10, 12]) and

$$(x \mapsto G(x,y) - \Phi(x,y)) \in H^1(\Omega)^{4\times4}.$$

Moreover, G can be differentiated in the second argument and we set

$$G^0(x) = G(x,0),\ \mathbf{G}^0(x) = D(-\nabla_y)G(x,y)|_{y=0}. \tag{101}$$

By repeating the considerations in and around of Lemma 3.1, we can detect that

$$G^0 - \Phi \in H^1(\Omega)^{4\times4},\ \mathbf{G}^0 - D(\nabla_x)\Phi - \mathbf{Z} - \mathbf{K}\Phi \in H^1(\Omega)^{9\times4}, \tag{102}$$

where $\mathbf{K}$ is a certain matrix of the size 9×4 with real entries and $\mathbf{Z}$ is such that $Z(x) = \mathbf{Z}(x)M^\top\varepsilon^0$ (cf. (73) and (75)-(77)). Since, by definition of $\mathbf{u}$ and S^q, the vector function $\mathbf{U}$ verifies the boundary conditions (95) and the homogeneous system (94) everywhere in Ω, except at the point O. Let us now compare singularities in (102) and (99) to conclude that

$$\mathbf{U}(x) = \mathbf{G}^0(x)M^\top\varepsilon^0 - G^0(x)f(0)mes_3\omega. \tag{103}$$

Remark 3.8. *1. We emphasize that the differential operator $D(-\nabla_y)$ in* (101) *is replaced by $D(\nabla_x)$ in* (102)*. This is due to the evident relationship $D(-\nabla_y)\Phi(x-y) = D(\nabla_x)\Phi(x-y)$.*

2. If A is a constant matrix, then the terms $\mathbf{Z}$ and $\mathbf{K}\Phi$ are absent in (102)*, in other words, their presence results from the variable coefficients of differential operator* (40)*. Therefore, the column $-f(0)mes_3\omega$ occurs on the right-hand side of* (103) *instead of the column* (84)*. To ensure that the additional column* (85) *does not effect the form of the last term in* (103)*, one may put $\varepsilon^0 = 0$ to see that then $J = 0$. A direct calculation leading to formula* (103) *can be found in* [39] *for the three-dimensional elasticity problem.*

Since the coordinate origin O is situated inside ω_h, i.e., outside $\overline{\Omega}_h$ (cf. Section 3.1), the second term (103) in the new ansatz (98) is smooth in the domain $\Omega(h)$, although the Green matrices (101) have singularities at O.

4. Justification of asymptotics and analysis of shape functionals

4.1. The justification of asymptotics.

The difference

$$\widetilde{u}^h = u^h - u - \chi(hw^1 + h^2w^2) - h^3\mathbf{u} \tag{104}$$

(see (42) and (98)) satisfies the integral identity

$$Q(\widetilde{u}^h, v; \Omega(h)) = \widetilde{\mathcal{F}}^h(v),\ v \in \mathring{H}^1(\Omega(h);\Gamma_u)^4, \tag{105}$$

where $\widetilde{\mathcal{F}}^h$ is a certain functional. If the estimate

$$|\widetilde{\mathcal{F}}^h| \le ch^{\alpha+5/2}\|v; H^1(\Omega(h))\| \tag{106}$$

is proved, we could take $v = \widetilde{u}^h$ in order to conclude by using (14) that

$$\|\widetilde{u}^h; H^1(\Omega(h))\| \le ch^{\alpha+5/2}. \tag{107}$$

To verify (106), first, we assume that v vanishes in the ball $\mathbb{B}_{2R/3}$ while $\chi v = 0$. Then, we have

$$\widetilde{\mathcal{F}}^h(v) = Q(u^h - u - h^3\mathbf{u}, v; \Omega(h)) = Q(u^h, v; \Omega(h)) - Q(u, v; \Omega) - h^3 Q(\mathbf{u}, v; \Omega). \tag{108}$$

Recalling (29), (12) and (96), we observe that the support of the vector function (91) satisfies $supp\, \mathbf{f} \subset \overline{\mathbb{B}}_{2R/3}$ and, hence, (108) is null.

Second, let $supp\, v \subset \mathbb{B}_R \setminus \omega_h$. We write

$$\begin{aligned} \widetilde{F}^h(v) &= (f, v)_{\Omega(h)} - (AD(\nabla_x)u, D(\nabla_x)v)_{\Omega(h)} - h^3(AD(\nabla_x)\mathbf{u}, D(\nabla_x)v)_{\Omega(h)} \\ &\quad - h(AD(\nabla_x)(\chi w^1), D(\nabla_x)v)_{\Omega(h)} - h^2(AD(\nabla_x)(\chi w^2), D(\nabla_x)v)_{\Omega(h)} \\ &=: (f, v)_{\Omega(h)} - I^u - h^3 I^{\mathbf{u}} - h I_1^w - h^2 I_2^w. \end{aligned} \tag{109}$$

Since the vector functions u and $\mathbf{u}$ are smooth in $\mathbb{B}_R \setminus \omega_h$, we integrate by parts and obtain

$$\begin{aligned} I^u &= (f, v)_{\Omega(h)} + (D(n^h)^\top A^0 \varepsilon^0, v)_{\partial\omega_h} + (D(n^h)^\top A^0 D(\nabla_x)U, v)_{\partial\omega_h} \\ &\quad + \sum_{j=1}^{3} (D(n^h)^\top x_j A^j \varepsilon^0, v)_{\partial\omega_h} + \widetilde{I}^u, \end{aligned} \tag{110}$$

$$\widetilde{I}^u = (D(n^h)^\top AD(\nabla_x)(u - D(x)^\top \varepsilon^0 - U), v)_{\partial\omega_h} +$$

$$(D(n^h)^\top (A - A^0 - \sum_{j=1}^{3} x_j A^j)\varepsilon^0, v)_{\partial\omega_h} + (D(n^h)^\top (A - A^0) D(\nabla_x)U, v)_{\partial\omega_h},$$

$$I^{\mathbf{u}} = (\mathbf{f}, v)_{\Omega(h)} + \widetilde{I}^{\mathbf{u}}, \quad \widetilde{I}^u = (D(n^h)^\top AD(\nabla_x)\mathbf{u}, v)_{\partial\omega_h}. \tag{111}$$

To process the terms $\widetilde{I}^u$ and $\widetilde{I}^{\mathbf{u}}$, we recall the inequality

$$\int_{\Omega(h)} |x|^{-2} |v(x)|^2 dx \leq c \|v; H^1(\Omega(h))\|^2 , \tag{112}$$

which is a consequence of the one-dimensional Hardy inequality (cf. [35, §4.5]) and the trace inequality (see [21])

$$\int_{\partial\omega_h} |v(x)|^2 ds_x \leq ch \|v; H^1(\Omega(h))\|^2 , \tag{113}$$

where the constants c are independent of $h \in (0, h_0]$ and v.

Now by (113) and (97), we readily derive that

$$\begin{aligned} h^3 |\widetilde{I}^{\mathbf{u}}| \leq ch^3 h^{-1-\alpha} \int_{\partial\omega_h} |v(x)| ds_x &\leq ch^{2-\beta} (mes_2 \partial\omega_h)^{1/2} h^{1/2} \|v; H^1(\Omega(h))\| \\ &= Ch^{-\beta+7/2} \|v; H^1(\Omega(h))\|. \end{aligned} \tag{114}$$

Analogously, by means of (39), (34) and (113), we have

$$|\widetilde{I}^u| \leq c(h^{1+\alpha} + h^2 + h^2) \int_{\partial\omega_h} |v(x)| ds_x \leq ch^{\alpha+5/2} \|v; H^1(\Omega(h))\|. \tag{115}$$

We may choose $\beta = 1 - \alpha > 0$ in order to equalize the final exponents of h in (114) and (115).

Dealing with I_2^w, we write

$$
\begin{aligned}
I_2^w &= (AD(\nabla_x\chi)S^1, D(\nabla_x)v)_{\Omega(h)} - (AD(\nabla_x)S^1, D(\nabla_x\chi)v)_{\Omega(h)} \\
&+ (A^0 D(\nabla_x)w^2, D(\nabla_x)(\chi v))_{\Omega(h)} + \widetilde{I}_2^w,
\end{aligned}
\tag{116}
$$

$$
\begin{aligned}
\widetilde{I}_2^w &= (AD(\nabla_x\chi)(w^2 - S^1), D(\nabla_x)v)_{\Omega(h)} - (AD(\nabla_x\chi)(w^2 - S^1), D(\nabla_x\chi)v)_{\Omega(h)} \\
&+ ((A - A^0)D(\nabla_x)w^2, D(\nabla_x)(\chi v))_{\Omega(h)}.
\end{aligned}
\tag{117}
$$

Here, we detach $S^1(h^{-1}x)$ from $w^2(h^{-1}x)$ (cf. (89)) and commute twice the differential operator $D(\nabla_x)$ with the cut-off function χ (see (92)).

In view of (39) and (82), the absolute value of the last expression in (117), multiplied by h^2 according to the definition of I_2^w in (109), does not exceed the sum of the following two expressions:

$$
\begin{aligned}
&ch^2 \int\limits_{\Omega\setminus\mathbb{B}_R h} |x| h^{-1} \left(\frac{|x|}{h}\right)^{-3+\beta} |D(\nabla_x)(\chi(x)v(x))| dx \leq \\
&\leq ch^{4-\beta} \left(\int\limits_{Rh}^{diam\Omega} r^2 r^{-6+2\beta} r^2 dr \right)^{1/2} \|v; H^1(\Omega(h))\| \leq ch^{7/2} \|v; H^1(\Omega(h))\|
\end{aligned}
\tag{118}
$$

and

$$
\begin{aligned}
&ch^2 \int\limits_{\mathbb{B}_{Rh}\setminus\omega_h} |x| |D(\nabla_x)\widetilde{w}^2(h^{-1}x)| |D(\nabla_x)(\chi v)| dx \\
&\leq ch^2 Rh \left(\int\limits_{\mathbb{B}_R\setminus\omega} h^{-2} |D(\nabla_\xi)\widetilde{w}^2(\xi)|^2 d\xi h^3 \right)^{1/2} \|v; H^1(\Omega(h))\| \\
&\leq ch^{7/2} \|v; H^1(\Omega(h))\|.
\end{aligned}
\tag{119}
$$

The radius R is chosen such that $\mathbb{B}_R \supset \overline{\omega}$. Since the support of $|D(\nabla_x\chi)|$ belongs to the annulus $\overline{\mathbb{B}_{2R/3}} \setminus \mathbb{B}_{R/3}$ where, according to (82),

$$
|w^2(h^{-1}x) - S^1(h^{-1}x)| + |\nabla_x(w^2(h^{-1}x) - S^1(h^{-1}x))| \leq ch^{2-\beta},
$$

the remaining terms in (117), again after multiplication by h^2, are bounded by $ch^{4-\beta}\|v; H^1(\Omega)\|$ while we may set $\beta = 1/2$ to achieve the same exponent as in (118). In other words, for $p = 2$, we now have

$$
h^p |\widetilde{I}_p^w| \leq ch^{7/2} \|v; H^1(\Omega(h))\|. \tag{120}
$$

By formulae (72), (55) and (89), the similar argument leads to the estimate (120) for the remainder in the representation

$$
\begin{aligned}
&I_1^w = (AD(\nabla_x\chi)S^2, D(\nabla_x)v)_{\Omega(h)} - (AD(\nabla_x)S^2, D(\nabla_x\chi)v)_{\Omega(h)} + \\
&(A^0 D(\nabla_x)w^1, D(\nabla_x)(\chi v))_{\Omega(h)} + \textstyle\sum_{j=1}^3 (x_j A^j D(\nabla_x)w^1, D(\nabla_x)(\chi v))_{\Omega(h)} + \widetilde{I}_1^w.
\end{aligned}
\tag{121}
$$

Now, we are in position to conclude the estimate (106) for the functional $\widetilde{F}^h$ in (105), (108) and (109). To this end, we list several facts. First, the inner product $(f, v)_{\Omega(h)}$ on the right hand-side of (109) cancels the same product in (110). Second, the equality

$$(\mathbf{f}, \mathbf{v})_{\Omega(h)} = -(AD(\nabla_x \chi)(S^2 - S^1), D(\nabla_x)v)_{\Omega(h)} + (AD(\nabla_x)(S^2 - S^1), D(\nabla_x \chi)v)_{\Omega(h)}$$

is inherited from the definitions (91) and (92). Third, we make the coordinate dilation $x \mapsto \xi = h^{-1}x$ in the first couples of terms on the right hand-side of (116) and (121), simultaneously multiplying the terms by h^2 and h, respectively. Noting that $S^p(h^{-1}x) = h^p S^p(x)$, $p = 1, 2$, we see that these couples and $h^3(\mathbf{f}, \mathbf{v})_{\Omega(h)}$ annihilate. Finally, we recall the integral identities (52), serving for the problems (46) and (47), and after the substitutions $x \mapsto \xi$ and $v(\xi) \mapsto \chi(h\xi)v(h\xi)$, we detect all terms in the identities on the right hand-sides of (110), (116) and (121). Thus,

$$\widetilde{F}^h(v) = \widetilde{I}^u + h^3\widetilde{I}^{\mathbf{u}} + h\widetilde{I}^w_1 + h^2\widetilde{I}^w_2$$

and the inequality (106) holds true by virtue of (115), (114) and (120) with $p = 1, 2$. We notice that the lowest exponent $\alpha+5/2$ of h occurs in (115) because $\alpha \in (1/2, 1)$ and $\alpha + 5/2 \in (3, 7/2)$.

We now formulate the result.

Theorem 4.1. *Let all assumptions in Section 3.1 be valid, in particular, the inclusion* (32) *with* $\alpha \in (1/2, 1)$. *Then the solution* u^h *of the piezoelectricity problem* (25)-(28) *and its approximation constructed in Section 3 are in the relationship*

$$\|u^h - u - h^3\mathbf{u} - \chi(hw^1 + h^2w^2); H^1(\Omega(h))\| \le ch^{\alpha+5/2}N, \tag{122}$$

where the constant c *is independent of the parameter* $h \in (0, h_0]$ *and the right-hand sides* f, g *while*

$$N = \|f; L^2(\Omega)\| + \|g; L^2(\partial\Omega)\| + \|f; C^{2,\alpha}(\mathbb{B}_R)\|. \tag{123}$$

Remark 4.2. *The obtained estimate* (122) *is asymptotically sharp, in particular, it satisfies the "first omitted term" rule. Indeed, for the smooth data* A *and* f, *the subsequent asymptotic term in the ansatz* (42) *is* $h^3\chi(x)w^3(h^{-1}x)$, *the* $H^1(\Omega(h))$*-norm of the latter term is just* $O(h^{7/2})$. *This bound appears in* (123) *if* $\alpha \to 1 - 0$. *Moreover, the estimate* (122) *holds true when the last addendum in* (123) *is changed for* $\|f; C^{3,\alpha_1}(\mathbb{B}_R)\|$ *with any* $\alpha_1 \in (0, 1)$. *If the right-hand side* $f \in C^{2,\alpha}(\mathbb{B}_R)^4$ *in the equations* (25) *is not sufficiently smooth, e.g.,*

$$f(x) = f^0(x) + |x|^{2+\alpha} f^1(\theta),\ f^0 \in C^\infty(\mathbb{B}_R)^4,\ f^1 \in C^\infty(\mathbb{S}_1)^4,$$

then the asymptotic ansatz (42) *gains the boundary layer term* $h^{2+\alpha}\chi(x)w^{2+\alpha}(h^{-1}x)$ *with the Sobolev norm in* $\Omega(h)$ *of the some order* $h^{\alpha+5/2}$ *as on the right hand-side of* (122).

A direct calculation show that

$$h^j\|\chi w^j; H^1(\Omega(h))\| = O(h^{j+1/2}),\ j = 1, 2, \tag{124}$$

and, therefore, in view of the relation $\alpha + 5/2 > 3$ (see (32)), the $H^1(\Omega(h))$-norm of each of the detached asymptotic terms in (122) (cf. (42) and (98)) is of order h^s

with $s \le 3$. In other words, Theorem 4.1 justifies the constructed asymptotics of solution u^h, indeed.

4.2. **The energy and the electric enthalpy.** We proceed with energy functional (17), assuming for simplicity that the volume forces and the volume charges are absent, i.e., $f = 0$ on the right hand-sides of (9) and (25). Then, integrating by parts and taking into account formulae (98) and (107), we have

$$\begin{aligned} \mathcal{U}(u^h;\Omega(h)) &= \tfrac{1}{2}(D(n)^\top AD(\nabla_x)u^h, u^h)_{\Gamma_\sigma} - (g, u^h)_{\Gamma_\sigma} = -\tfrac{1}{2}(g, u^h)_{\Gamma_\sigma} \\ &= -\tfrac{1}{2}(g, u)_{\Gamma_\sigma} - \tfrac{1}{2}h^3(g, \mathbf{u})_{\Gamma_\sigma} + O(h^{\alpha+5/2})\,. \end{aligned} \tag{125}$$

Let $\mathfrak{v}^{\mathsf{M}} \in \mathring{H}^1(\Omega;\Gamma_u)^4$ and $\mathfrak{v}^{\mathsf{E}} \in \mathring{H}^1(\Omega;\Gamma_u)^4$ imply the solutions of the problem (9)-(11) with the right-hand sides

$$\mathfrak{g}^{\mathsf{M}} = (g_1^{\mathsf{M}}, g_2^{\mathsf{M}}, g_2^{\mathsf{M}}, 0)^\top,\ \mathfrak{g}^{\mathsf{E}} = (0,0,0,g_4^{\mathsf{E}})^\top. \tag{126}$$

Using the representation (103) with $f(0) = 0$ and the modified column $\mathbf{U}_{(-)}$ (see (65)), we obtain

$$\begin{aligned} (\mathfrak{g}^{\mathsf{M}}, \mathbf{U})_{\Gamma_\sigma} &= (\mathfrak{g}^{\mathsf{M}}, \mathbf{U}_{(-)})_{\Gamma_\sigma} = (D(n)^\top AD(\nabla_x)\mathfrak{v}^{\mathsf{M}}, \mathbf{U}_{(-)})_{\Gamma_\sigma} \\ &= (\mathfrak{v}^{\mathsf{M}}, D(-\nabla_x)^\top A^\top D(\nabla_x)\mathbf{U}_{(-)})_{\Gamma_\sigma} \\ &= (\varepsilon^0)^\top M(\mathfrak{v}^{\mathsf{M}}, D(-\nabla_x)^\top A^\top D(\nabla_x)\mathbf{G}^0_{(-)})_\Omega \\ &= (\varepsilon^0)^\top M(\mathfrak{v}^{\mathsf{M}}, (D(\nabla_x)^\top \delta(x))_{(-)})_\Omega = -(\varepsilon^0)^\top M\mathfrak{e}^{\mathsf{M}}_{(-)}, \\ (\mathfrak{g}^{\mathsf{E}}, \mathbf{U})_{\Gamma_\sigma} &= (\mathfrak{g}^{\mathsf{E}}, \mathbf{U}_{(-)})_{\Gamma_\sigma} = -(\mathfrak{v}^{\mathsf{E}}, D(-\nabla_x)^\top A^\top D(\nabla_x)\mathbf{U}_{(-)})_{\Gamma_\sigma} \\ &= (\varepsilon^0)^\top M\mathfrak{e}^{\mathsf{E}}_{(-)}. \end{aligned} \tag{127}$$

Here, we apply formula (100) for the derivatives $\mathbf{G}^0$ of the Green matrix G in (100). We emphasize that

$$(f, \mathbf{G}^0_{(-)})_\Omega + (g, \mathbf{G}^0_{(-)})_{\Gamma_\sigma} = -(D(\nabla_x)u)_{(-)}(0) = -\varepsilon^0_{(-)} \tag{128}$$

because entries of $\mathbf{G}^0$ are given by the derivatives of columns of the fundamental matrix $G(x,y)$ with respect to the second argument, and $G_{(-)}$ satisfies the problem

$$\begin{aligned} &D(-\nabla_x)^\top A(x)^\top D(\nabla_x)G_{(-)}(x,y) = \delta(x-y)\mathbb{I}_{(-)},\ x \in \Omega, \\ &D(n(x))^\top A(x)^\top D(\nabla_x)G_{(-)}(x,y) = 0,\ x \in \Gamma_\sigma,\ G_{(-)}(x,y) = 0,\ x \in \Gamma_u, \end{aligned}$$

where $\mathbb{I}_{(-)} = diag\{1,1,1,-1\}$ (cf. the problem (100)).

By (125) and (127), the following representation is valid:

$$\mathcal{U}(u^h;\Omega(h)) - \mathcal{U}(u;\Omega) = \frac{h^3}{2}(\varepsilon^0)^\top M(\mathfrak{G}^{\mathsf{M}}_{(-)} - \mathfrak{G}^{\mathsf{E}}_{(-)}) + O(h^{\alpha+5/2}). \tag{129}$$

At the first sight, (129) looks like (1), however this impression is wrong.

Remark 4.3. *The decomposition $u = \mathfrak{v}^{\mathsf{M}} + \mathfrak{v}^{\mathsf{E}}$ is only a mathematical device in our analysis, since in a smart material it is impossible to distinguish between the strain columns $\mathfrak{e}^{\mathsf{M}} = D(\nabla_x)\mathfrak{v}^{\mathsf{M}}(0)$ and $\mathfrak{e}^{\mathsf{E}} = D(\nabla_x)\mathfrak{v}^{\mathsf{E}}(0)$ generated at the point O by the external mechanical loading $\mathfrak{g}^{\mathsf{M}}$ and the electrical surface charge $\mathfrak{g}^{\mathsf{E}}$ in* (126). *Surely, one can measure only the sum $\varepsilon^0 = D(\nabla_x)u(0)$ resulting from complete external action and standing as the first term on the right hand-side of* (129).

The difference

$$\mathfrak{e}^{\mathsf{M}} - \mathfrak{e}^{\mathsf{E}} = (\mathfrak{g}^{\mathsf{E}}, \mathbf{G}^0)_{\Gamma_\sigma} - (\mathfrak{g}^{\mathsf{M}}, \mathbf{G}^0)_{\Gamma_\sigma}$$

ought to be regarded as a global characteristics of the mechanical electric state of the body Ω and, therefore, formula (129) has a different physical meaning compared to (1) and (136) below.

Remark 4.4. *A similar situation with the energy functional occurs for a crack in a piezoelectric medium. Applying the Griffith energy fracture criterion, in* [42] *the energy release rate at the crack tip is expressed in terms of stress intensity factors, i.e., local characteristics of the elastic/electric state at the tip. In* [20] *a mistake in a calculation (formulas (33.23) and (34.48) in* [42, pages 296 and 312]*; cf. comments in* [20]*) was discovered and a non-local formula for the energy release rate of type* (129) *was derived rigourously and justified. The non-local character of the energy release rate means that the energy functional* $\mathcal{U}(u;\Omega)$ *cannot be employed for a fracture criterion and in the Griffith criterion must involve the electric enthalpy (cf.* [14, 42] *for an interpretation from the view point of solid mechanics).*

Let us now compute the increment $\mathcal{E}(u^h;\Omega(h)) - \mathcal{E}(u;\Omega)$ of the mechanical enthalpy determined in (20) and (21). Returning back to the general case $f \neq 0$, we obtain

$$\begin{aligned} &\mathcal{E}(u^h;\Omega(h)) = \tfrac{1}{2}(AD(\nabla_x)u^h, D(\nabla_x)u^h_{(-)})_{\Omega(h)} - (f, u^h_{(-)})_\Omega - (g, u^h_{(-)})_\Omega \\ &= \tfrac{1}{2}(D(-\nabla_x)^\top AD(\nabla_x)u^h, u^h_{(-)})_{\Omega(h)} + \tfrac{1}{2}(D(n)^\top AD(\nabla_x)u^h, u^h_{(-)})_{\Gamma_\sigma} \\ &-(f, u^h_{(-)})_\Omega - (g, u^h_{(-)})_\Omega = -\tfrac{1}{2}(f, u^h_{(-)})_\Omega - \tfrac{1}{2}(g, u^h_{(-)})_{\Gamma_\sigma}. \end{aligned} \tag{130}$$

As above, we have

$$(g, u^h_{(-)})_{\Gamma_\sigma} = (g, u_{(-)})_{\Gamma_\sigma} + h^3(g, \mathbf{U}_{(-)})_{\Gamma_\sigma} + O(h^{\alpha+5/2}). \tag{131}$$

Furthermore, in view of representation (98) we derive

$$(f, u^h_{(-)})_{\Gamma_\sigma} = (f, u_{(-)})_{\Gamma_\sigma} + h^3(f, \mathbf{U}_{(-)})_{\Gamma_\sigma} + O(h^{\alpha+5/2}). \tag{132}$$

according to inequality (107) and the following relations

$$h^3|(f, \mathbf{U}_{-})_{\omega_h}| \leq ch^3 \int\limits_{\omega_h} |x|^{-2} dx \leq ch^4 \leq ch^{\alpha+5/2},$$

$$h|(f, \chi\widetilde{w}^1)_{\Omega(h)}| \leq ch \int\limits_0^{diam\Omega} (1 + \frac{r}{h})^{-3} r^2 dr \leq ch^4 |\ln h| \leq ch^{\alpha+5/2}, \tag{133}$$

$$h^2|(f, \chi\widetilde{w}^2)_{\Omega(h)}| \leq ch^2 \int\limits_0^{diam\Omega} (1 + \frac{r}{h})^{-2+\delta} r^2 dr \leq ch^{4-\delta} \leq ch^{\alpha+5/2}. \tag{134}$$

In the estimation (133) we have used the formulae (55) and (82) for $\widetilde{w}^1$ and $\widetilde{w}^2$ together with the demanded inclusions $\alpha \in (1/2, 1)$ and $\delta \in (0, 1/2)$.

Now formulae (131), (132) and (103), (128) convert (130) into the form

$$
\begin{aligned}
(135)\qquad & \mathcal{E}(u^h;\Omega(h)) - \mathcal{E}(u;\Omega) = -\tfrac{1}{2}(f, u_{(-)})_{\omega_h} + \\
& +\tfrac{1}{2}h^3 f(0)^\top mes_3\omega((f, G^0_{(-)})_\Omega + (g, G^0_{(-)})_{\Gamma_\sigma}) - \\
& -\tfrac{1}{2}h^3(\varepsilon^0)^\top M((f, \mathbf{G}^0_{(-)})_\Omega + (g, \mathbf{G}^0_{(-)})_{\Gamma_\sigma}) + O(h^{\alpha+5/2}) = \\
& -\tfrac{1}{2}((f, u_{(-)})_{\omega_h} - u_-(0)^\top f(0) mes_3\omega_h) + \tfrac{1}{2}h^3(\varepsilon^0)^\top M\varepsilon^0_{(-)} + O(h^{\alpha+5/2}) \\
& = \tfrac{1}{2}h^3(\varepsilon^0)^\top M_{(=)}\varepsilon^0 + O(h^{\alpha+5/2}).
\end{aligned}
$$

Here, we have taken into account that, first, $M\varepsilon^0_{(-)} = M_{(=)}\varepsilon^0$ according to the definition of $M_{(=)}$ in (63) and, second, $u_-(0)^\top f(0) mes_3\omega_h = (f, u_{(-)})_{\omega_h} + O(h^{3+\alpha})$ due to the smoothness properties (33) and (34) of f and u.

Let us formulate the result obtained in (135).

Theorem 4.5. *The electrical enthalpy* (20) *admits the asymptotic expansion*

$$
(136)\qquad \mathcal{E}(u^h;\Omega(h)) = \mathcal{E}(u;\Omega) + \frac{1}{2}h^3(\varepsilon^0)^\top M_{(=)}\varepsilon^0 + O(h^{\alpha+5/2}),
$$

where u^h and u imply solutions of the piezoelectricity problems (25)-(28) *and* (9)-(11)*, respectively, $\varepsilon^0 = D(\nabla_x)u(0)$ is the strain column* (35) *and $M_{(=)} = M_{(=)}(A^0, \omega)$ is the modified polarization matrix which is a symmetric matrix of size* 9×9 *(see formulae* (62), (63) *and Theorem 3.4).*

Note that in contrast to the energy functional (16) the electrical enthalpy has the topological derivative

$$
(137)\qquad \frac{1}{2}(D(\nabla_x)u(0))^\top M_{(=)}(A^0, \omega_h)D(\nabla_x)u(0)
$$

expressed in terms of local characteristics of the elastic/electric state in the entire body Ω and of the shape of the small void ω_h. Owing to representation (64), we emphasize that the polarization matrix (62) enjoys the homogeneity property $M(A^0;\omega_h) = h^3 M(A^0;\omega_h)$ which has been used in the passage from (136) to (137).

4.3. **Shape functionals and the adjoint state.** Recalling the Sobolev embedding theorem $H^1(\Omega) \subset L^6(\Omega)$ in $\mathbb{R}^3$, we assume that the density J in the shape functional

$$
(138)\qquad \mathcal{J}(u;\Omega) = \int_\Omega J(u(x);x)dx
$$

satisfies the following restrictions:

$$
(139)\qquad |J(a;x)| \le c(1 + |a|^t),
$$

$$
(140)\qquad |J(b;x) - J(a;x) - J'(a;x)^\top(b-a)| \le c|a-b|^2(1 + |a|^{t-1} + |b|^{t-1}),
$$

$$
(141)\qquad |J(b;x) - J(b;0)| \le c|x|^\gamma(1 + |b|^t)
$$

where $x \in \Omega$, a and b are arbitrary columns in $\mathbb{R}^4$, and the vector function J' is subject to the conditions

$$
(142)\qquad |J'(a;x)| \le c(1 + |a|^{t-1}),
$$

$$
(143)\qquad |J'(a;x) - J'(b;y)| \le c(|a-b|^\gamma(|a|^{t-\gamma} + |b|^{t-\gamma}) + |x-y|^\gamma(|a|^t + |b|^t)),
$$

while

$$t \in [2,6),\ \gamma \in (0,1). \tag{144}$$

In other words, along with the restrictions on the growth of J and J', the integrand J is differentiable with respect to the first variable and Hölder continuous with respect to the second variable. Moreover, J' is Hölder continuous in both arguments. Inequality (139) ensure that functional (138) is defined for $u \in H^1(\Omega)^4 \subset L^6(\Omega)^4 \subset L^t(\Omega)^4$.

We consider the difference

$$\mathcal{J}(u^h;\Omega(h)) - \mathcal{J}(u;\Omega) = \int\limits_{\Omega(h)} (J(u^h(x);x) - J(u(x);x))dx + \int\limits_{\omega_h} J(u(x);x)dx. \tag{145}$$

and, owing to (140) and (98), obtain the formula

(146)
$$\begin{aligned}|J(u^h(x);x) - J(u(x);x) - J'(u(x);x)^\top (h^3\mathbf{U}(x) + \chi(x)\textstyle\sum_{j=1}^2 h^j \widetilde{w}^j(\frac{x}{h}) + \widetilde{u}^h(x))| \leq \\ \leq c(h^2|\mathbf{U}(x)|^2 + \chi(x)^2 \textstyle\sum_{j=1}^2 h^{2j}|\widetilde{w}^j(\frac{x}{h})|^2 + |\widetilde{u}^h(x)|^2)(1 + |u^h(x)|^{t-2} + |u(x)|^{t-2}).\end{aligned}$$

Recalling the estimates (107), (142) and applying the Hölder inequality with the index couples $(p,q) = (5/6, 6)$ and $(p,q) = (3, 2/3)$, we obtain

$$\begin{aligned}\int\limits_{\Omega(h)} J'(u(x);x)^\top \widetilde{u}^h(x)dx \leq c\int\limits_{\Omega(h)} (1 + |u(x)|^5)|\widetilde{u}^h(x)|dx \leq \\ \leq c(1 + \|u;L^6(\Omega)\|^5)\|\widetilde{u}^h;L^6(\Omega(h))\| \leq c\|\widetilde{u}^h;H^1(\Omega)\| \leq ch^{\alpha+5/2}, \\ \int\limits_{\Omega(h)} |\widetilde{u}^h|^2(1 + |u^h|^{t-2} + |u|^{t-2})dx \leq c\int\limits_{\Omega(h)} |\widetilde{u}^h|^2(1 + |u^h|^4 + |u|^4)dx \leq \\ \leq c\|\widetilde{u}^h;L^6(\Omega(h))\|^2(1 + \|u^h;L^6(\Omega(h))\|^4 + \|u;L^6(\Omega)\|^4) \leq ch^{2\alpha+5}.\end{aligned}$$

Similarly,

$$h^6 \int\limits_{\Omega\setminus\mathbb{B}'_R} |\mathbf{U}(x)|^2(1 + |u^h(x)|^{t-2} + |u(x)|^{t-2})dx \leq ch^6.$$

However, because of the singularity $|\mathbf{U}(x)| = O(|x|^{-2})$, we use in the ball $\mathbb{B}_{R'}$ the Hölder inequality with the couple

$$(p,q) = \left(\frac{6}{8-t}, \frac{6}{t-2}\right) \tag{147}$$

to derive that

$$\begin{aligned}h^6 \int\limits_{\mathbb{B}_{R'}\setminus\omega_h} |\mathbf{U}|^2(1 + |u^h|^{t-2} + |u|^{t-2})dx \leq ch^6 \left(\int\limits_{ch}^{R'} r^{-\frac{24}{8-t}} r^2 dr\right)^{\frac{8-t}{6}} \times \\ \times(1 + \|u^h;H^1(\Omega(h))\|^{t-2} + \|u;H^1(\Omega)\|^{t-2}) \leq ch^{6-t/2}.\end{aligned}$$

We deal with the boundary layers in the same way as in (118) and (119). Outside the ball $\mathbb{B}_{Rh}$ we apply the inequalities (55) and (82) even much rougher ones, to conclude by the Hölder inequality with the index couple (147) that

$$
\begin{aligned}
&h^{2j} \int\limits_{\Omega\setminus\mathbb{B}_{Rh}} \left|\chi(x)\widetilde{w}^j\left(\frac{x}{h}\right)\right|^2 (1+|\widetilde{u}^h(x)|^2+|u(x)|^2)dx \le \\
&\le ch^6 \left(\int\limits_{ch}^{R'} r^{-\frac{12(3-j)}{8-t}} r^2 dr\right)^{\frac{8-t}{6}} \le ch^{6-t/2},\ j=1,2.
\end{aligned} \tag{148}
$$

Inside the ball $\mathbb{B}_{Rh}$ the Hölder inequality gives

$$
\begin{aligned}
h^{2j} &\int\limits_{\mathbb{B}_{Rh}\setminus\omega_h} \left|\widetilde{w}^j\left(\frac{x}{h}\right)\right|^2 (1+|\widetilde{u}^h(x)|^2+|u(x)|^2)dx \\
&\le ch^{2j}\left(\int\limits_{\mathbb{B}_{Rh}\setminus\omega_h} |\widetilde{w}^j\left(\frac{x}{h}\right)|^{\frac{12}{8-t}}dx\right)^{\frac{8-t}{6}} = ch^{2j+3\frac{8-t}{6}}\left(\int\limits_{\mathbb{B}_{Rh}\setminus\omega} \widetilde{w}^j\left(\frac{x}{h}\right)|^{\frac{12}{8-t}}d\xi\right)^{\frac{8-t}{6}} \\
&\le ch^{2j+4-t/2} \le ch^{6-t/2},\ j=1,2.
\end{aligned}
$$

Note that $\frac{12}{8-t} < 6$ due to (144) and, therefore,

$$
\|\widetilde{w}^j; L^{\frac{12}{8-t}}(\mathbb{B}_R\setminus\omega)\| \le c\|\widetilde{w}^j; H^1(\mathbb{B}_R\setminus\omega)\| \le c\|\widetilde{w}^j; V_0^1(\Xi)\|.
$$

Although, the faster rates of decay of the remainders $\widetilde{w}^1$ and $\widetilde{w}^2$ (cf. (89)) are not used in the estimation (148), the rate of decay becomes an important ingredient of the inequalities

$$
h^j\left|\int\limits_{\Omega(h)} J'(u(x);x)^\top \chi(x)\widetilde{w}^j\left(\frac{x}{h}\right)dx\right| \le ch^{7/2},\ j=1,2,
$$

its derivation is much simpler, though. A simplification originates from the relation $|J'(u(x);x)| \le const$ for $x \in supp\chi \subset \mathbb{B}_{R'}$ so that one may repeat the calculation (133).

Finally, we write

$$
h^3\left|\int\limits_{\omega_h} J'(u(x);x)^\top \mathbf{U}(x)dx\right| \le ch^3\int\limits_0^{Rh} r^{-2}r^2dr \le ch^4
$$

and, in view of (34) and (143),

$$
\left|\int\limits_{\omega_h} J(u(x);x)dx - h^3 J(u(0);0)mes_3\omega\right| \le ch^{3+min\{\alpha,\gamma\}}
$$

Everything is prepared to derive a formula of type (1) for the shape functional (138).

Theorem 4.6. *Let the assumption formulated above hold true. Then the asymptotic formula*

$$\begin{aligned}\mathcal{J}(u^h;\Omega(h)) &= \mathcal{J}(u;\Omega) + h^3((J(u(0);0) - P(0)^\top f(0))mes_3\omega \\ &- (D(\nabla_x)P(0))^\top M\varepsilon^0) + O(h^{3+min\{\gamma,\alpha-1/2,3-t/2\}})\end{aligned} \tag{149}$$

is valid where $P \in \mathring{H}^1(\Omega;\Gamma_u)^4 \cap C^{2,min\{\alpha,\gamma\}}(\mathbb{B}_{R'})^4$ *is a solution of the formally adjoint piezoelectricity problem*

$$\begin{aligned}&D(-\nabla_x)^\top A(x)^\top D(\nabla_x)P(x) = J'(u(x);x),\ x \in \Omega,\\ &D(n(x))^\top A(x)^\top D(\nabla_x)P(x) = 0,\ x \in \Gamma_\sigma, P(x) = 0,\ x \in \Gamma_\sigma.\end{aligned} \tag{150}$$

Proof. The calculations performed above provide the relation

$$h^{-3}(\mathcal{J}(u^h;\Omega(h)) - \mathcal{J}(u;\Omega)) = J(u(0);0)mes_3\omega + (J'(u),\mathbf{U})_\Omega + O(h^{min\{\gamma,\alpha-1/2,3-t/2\}}).$$

We recall the representation (103) where G^0 is the Green matrix, i.e., a solution to the problem (100). The Green matrix and derivatives help to calculate the solution P of the formally adjoint problem (150) and the derivatives $\mathbf{G}^0$ (see (101)) deliver the column $D(\nabla_x)P(x)$ at the point $x = 0$. In other words, we write

$$\begin{aligned}(J'(u),\mathbf{U})_\Omega &= (D(-\nabla_x)^\top A(x)^\top D(\nabla_x)P, \mathbf{G}^0)_\Omega M\varepsilon^0 - mes_3(\omega G^0 f(0))_\Omega\\ &= (P, D(\nabla_x)^\top \delta M\varepsilon^0)_\Omega - mes_3\omega(P,\delta f(0))_\Omega\\ &= -(D(\nabla_x)P(0))^\top M\varepsilon^0 - P(0)^\top f(0)mes_3\omega.\end{aligned} \tag{151}$$

We again used the Dirac measure δ in the framework of the theory of distributions to compute the expression (151).

Finally, in order to justify our calculations we make the following comments. By assumptions (139), (144) and (143), (32), the functional

$$\mathring{H}^1(\Omega;\Gamma_u)^4 \ni v \to (J'(u),v)_\Omega$$

is continuous and $J'(u) \in C^{0,min\{\alpha,\gamma\}}(\mathbb{B}_{R'})$ with any $R' < R$. Thus, the same arguments as in Sections 2.3 and 3.1 guarantee the existence of a solution P to the problem (150) which is twice differentiable in the vicinity of the point $x = 0$. These observations make all calculations justified.■

The topological derivative of the functional $\mathcal{J}$, i.e.,

$$\mathcal{T}(u,\omega) = (J(u(0);0) - P(0)^\top f(0))mes_3\omega - (D(\nabla_x)P(0))^\top M\varepsilon^0,$$

is non-local since it involves the adjoint state P in (150) which depends on the solution u of the piezoelectricity problem in the entire domain Ω.

4.4. **Example.** Assume that there is a weak interaction between the mechanical and electric fields. This means that in the decomposition

$$A = A_{(0)} + A_{(1)}\ , \tag{152}$$

$$A_{(0)} = \begin{pmatrix} A^{\mathsf{MM}} & \mathbb{O}_{6\times3} \\ \mathbb{O}_{3\times6} & A^{\mathsf{EE}} \end{pmatrix},\quad A_{(1)} = \begin{pmatrix} \mathbb{O}_{6\times6} & -A^{\mathsf{ME}} \\ A^{\mathsf{EM}} & \mathbb{O}_{3\times3} \end{pmatrix}$$

the entries of matrix $A_{(1)}$ are much smaller compared to non trivial entries of the matrix $A_{(0)}$. It implies that in the first order approximation the piezoelectricity problem is decoupled into two problems, the pure elasticity problem with the stiffness matrix A^{MM}, and the pure electricity problem with the permeability matrix A^{EE}.

We are going to evaluate the main correction terms in the asymptotic expansions of characteristics for the piezoelectric bodies Ω, Ξ and $\Omega(h)$ (see Sections 2.2, 3.3 and 3.1). We proceed with the solution

$$u(x) = u_{(0)} + u_{(1)}(x) + \dots \tag{153}$$

of the problem (9)-(11). In (153) and further, the dots stand for the second order terms. In view of (152), the displacement vector $u^{\mathsf{M}}_{(0)}$ and the electric vector $u^{\mathsf{E}}_{(0)}$ verify the problems

$$D^{\mathsf{M}}(-\nabla_x)^\top A^{\mathsf{MM}}(x) D^{\mathsf{M}}(\nabla_x) u^{\mathsf{M}}_{(0)}(x) = f^{\mathsf{M}}(x),\ x \in \Omega, \tag{154}$$
$$D^{\mathsf{M}}(n(x))^\top A^{\mathsf{MM}}(x) D^{\mathsf{M}}(\nabla_x) u^{\mathsf{M}}_{(0)}(x) = g^{\mathsf{M}}(x),\ x \in \Gamma_\sigma, \quad u^{\mathsf{M}}_{(0)}(x) = 0,\ x \in \Gamma_u,$$

$$-\nabla_x^\top A^{\mathsf{EE}} \nabla_x u^{\mathsf{E}}_{(0)}(x) = f^{\mathsf{E}}(x),\ x \in \Omega, \tag{155}$$
$$n^\top A^{\mathsf{EE}} u^{\mathsf{E}}_{(0)}(x) = g^{\mathsf{E}}(x),\ x \in \Gamma_\sigma, \quad u^{\mathsf{E}}_{(0)}(x) = 0,\ x \in \Gamma_u\ ,$$

and can be determined separately. Inserting (153) and (152) into (9)- (11), we arrive at the problem

$$\begin{gathered} D(-\nabla_x)^\top A_{(0)}(x) D(\nabla_x) u_{(1)}(x) = D(-\nabla_x)^\top A_{(1)}(x) D(\nabla_x) u_{(0)}(x),\ x \in \Omega, \\ D(n(x))^\top A_{(0)}(x) D(\nabla_x) u_{(1)}(x) = D(n(x))^\top A_{(1)}(x) D(\nabla_x) u_{(0)}(x),\ x \in \Gamma_\sigma, \\ u_{(1)}(x) = 0,\ x \in \Gamma_u\ . \end{gathered} \tag{156}$$

This problem is decoupled as well, however, its solution manifests the interaction between electric and mechanical fields, since the displacement vector $u^{\mathsf{M}}_{(1)}$ depends only on the main part $u^{\mathsf{E}}_{(0)}$ of the electric potential and, in the same manner, $u^{\mathsf{E}}_{(1)}$ depends on $u^{\mathsf{M}}_{(0)}$.

In order to complete the asymptotic formulae, in the same way as in the previous sections, we also need the expansion for the polarization matrix

$$M = M_{(0)} + M_{(1)} + \dots\ , \tag{157}$$
$$M_{(0)} = \begin{pmatrix} M^{\mathsf{M}} & \mathbb{O}_{6\times3} \\ \mathbb{O}_{3\times6} & M^{\mathsf{E}} \end{pmatrix}, \quad M_{(1)} = \begin{pmatrix} \mathbb{O}_{6\times6} & M^{\mathsf{ME}} \\ M^{\mathsf{EM}} & \mathbb{O}_{3\times3} \end{pmatrix}.$$

We emphasize that the matrices $M_{(0)}$ and $M_{(1)}$ inherit the block diagonal structure of $A_{(0)}$ and the block-anti-diagonal of $A_{(1)}$, respectively. The same structures are kept by all matrix objects, in particular, the fundamental matrix takes the form

$$\Phi = \Phi_{(0)} + \Phi_{(1)} + \dots\ , \tag{158}$$
$$\Phi_{(0)} = \begin{pmatrix} \Phi^{\mathsf{M}} & \mathbb{O}_{3\times1} \\ \mathbb{O}_{1\times3} & \Phi^{\mathsf{E}} \end{pmatrix}, \quad \Phi_{(1)} = \begin{pmatrix} \mathbb{O}_{3\times3} & \Phi^{\mathsf{ME}} \\ \Phi^{\mathsf{EM}} & 0 \end{pmatrix}.$$

Here, Φ^{M} is the fundamental matrix for the elasticity matrix operator $D^{\mathsf{M}}(-\nabla_\xi)^\top A^{0\mathsf{M}} D^{\mathsf{M}}(\nabla_\xi)$ and Φ^{E} is the fundamental matrix for the scalar operator $-\nabla_\xi^\top A^{0\mathsf{E}} \nabla_\xi$. Furthermore, M^{E} and M^{M} are the virtual mass matrix and the elasticity polarization matrix for the cavity $\omega \subset \mathbb{R}^3$, which are negative definite (see [44] and [34, 40]).

It is convenient to proceed with the matrix solution (60) which, according to (152) and (61), enjoys the expansion

$$W = W_{(0)} + W_{(1)} + \dots , \tag{159}$$
$$W_{(0)} = \begin{pmatrix} W^{\mathsf{M}} & \mathbb{O}_{3\times 3} \\ \mathbb{O}_{1\times 6} & W^{\mathsf{E}} \end{pmatrix} , \quad W_{(1)} = \begin{pmatrix} \mathbb{O}_{3\times 6} & W^{\mathsf{ME}} \\ W^{\mathsf{EM}} & \mathbb{O}_{1\times 3} \end{pmatrix}$$

with

$$W(\xi) = (MD(\nabla_\xi)\Phi(\xi)^\top)^\top + O(|\xi|^{-2}) = \tag{160}$$
$$(M_{(0)}D(\nabla_\xi)\Phi_{(0)}(\xi)^\top)^\top + (M_{(0)}D(\nabla_\xi)\Phi_{(1)}(\xi)^\top + M_{(1)}D(\nabla_\xi\Phi_{(0)}(\xi)^\top)^\top + \dots + O(|\xi|^{-2}) .$$

The correction term $\Phi_{(1)}$ in (158) is a power-law solution of form (76) for the system of differential equations

$$D(-\nabla_\xi)^\top A^0_{(0)} D(\nabla_\xi)\Phi_{(1)}(\xi) = D(\nabla_\xi)^\top A^0_{(1)} D(\nabla_\xi)\Phi_{(0)}(\xi) , \quad \xi \in \mathbb{R}^3 \setminus \{0\} , \tag{161}$$

(cf. (77)). By a general result in [18] (see also [35, Lemmas 3.3.1 and 3.5.11]), the solution $\Phi_{(1)}$ can depend linearly on $\ln|\xi|$, however, the same argument as in the proof of Lemma 3.1 ensures that $\Phi_{(1)}$ is positive homogeneous of degree -1 according to (53). The solution $\Phi_{(1)}$, which is defined up to the linear combination $\Phi_{(0)}C$ of the fundamental matrix columns with the constant column $C \in \mathbb{R}^4$, can be fixed such that

$$\int_{\mathbb{S}_\varkappa} D(\nabla_\xi)^\top A^0 D(\nabla_\xi)\Phi_{(1)}(\xi) ds_\xi = 0 \in \mathbb{R}^4 . \tag{162}$$

The exterior problem for the correction term in (159) takes the form

$$D(-\nabla_\xi)^\top A^0_{(0)} D(\nabla_\xi) W_{(1)}(\xi) = D(\nabla_\xi)^\top A^0_{(1)} D(\nabla_\xi) W_{(0)}(\xi) , \xi \in \Xi , \tag{163}$$
$$D(n^\omega(\xi))^\top A^0_{(0)} D(\nabla_\xi) W_{(1)}(\xi) = -D(n^\omega(\xi))^\top A^0_{(1)} D(\nabla_\xi) W_{(0)}(\xi) , \xi \in \partial\omega . \tag{164}$$

Since, owing to (160), we have

$$W_{(0)}(\xi) = (M_{(0)} D(\nabla_\xi)\Phi_{(0)}(\xi)^\top)^\top + O(|\xi|^{-3}) ,$$

the right-hand side $F_{(1)}(\xi)$ in (163) admits the decomposition

$$
\begin{aligned}
F_{(1)}(\xi) &= D(\nabla_\xi)^\top A^0_{(1)} D(\nabla_\xi)(D(\nabla_\xi)\Phi_{(0)}(\xi)^\top)^\top M^\top_{(0)} + \widetilde{F}_{(1)}(\xi) = \\
&= \sum_{q=1}^{3} \frac{\partial}{\partial \xi_q} D(\nabla_\xi)^\top A^0_{(1)} D(\nabla_\xi)\Phi_{(0)}(\xi)^\top D(e_q)^\top M^\top_{(0)} + \widetilde{F}_{(1)}(\xi) = \\
&= \sum_{q=1}^{3} D(-\nabla_\xi)^\top A^0_{(0)} D(\nabla_\xi) \frac{\partial \Phi_{(1)}}{\partial \xi_q} D(e_q)^\top M^\top_{(0)} + \widetilde{F}_{(1)}(\xi)
\end{aligned}
\tag{165}
$$

with the remainder $\widetilde{F}_{(1)}(\xi) = O(|\xi|^{-5})$. In (165), the equation (161) has been applied. Comparing (165) with (160), we set

$$
W_{(1)}(\xi) = \widetilde{W}_{(1)}(\xi) + (M_{(0)} D(\nabla_\xi)\Phi_{(0)}(\xi)^\top)^\top \ . \tag{166}
$$

Recall that ω contains the origin $\xi = 0$, therefore, the last term in (166) is smooth in $\overline{\Xi}$. As a result, a new exterior problem is obtained, with the right-hand side $\widetilde{F}_{(1)}$ which decays sufficiently fast at infinity,

$$
\begin{aligned}
D(-\nabla_\xi)^\top A^0_{(0)} D(\nabla_\xi)\widehat{W}_{(1)}(\xi) &= \widetilde{F}_{(1)}(\xi) \ , \xi \in \Xi \ , \\
D(n^\omega(\xi))^\top A^0_{(0)} D(\nabla_\xi)\widehat{W}_{(1)}(\xi) &= \widetilde{G}_{(1)}(\xi) \ , \xi \in \partial\omega \ ,
\end{aligned}
\tag{167}
$$

where

$$
\begin{aligned}
\widetilde{G}_{(1)}(\xi) &= D(n^\omega(\xi))^\top A^0_{(1)} D(\nabla_\xi)\widehat{W}_{(0)}(\xi) - \\
&- D(n^\omega(\xi))^\top A^0_{(0)} D(\nabla_\xi)(M_{(0)} D(\nabla_\xi)\Phi_{(1)}(\xi)^\top)^\top \ .
\end{aligned}
\tag{168}
$$

Now, the decay of $\widetilde{G}_{(1)}(\xi)$ can be used, indeed, by Proposition 3.2 (see [18] and [35, Theorem 3.5.6]) and the calculations (57), (56), the solution $\widehat{W}_{(1)} \in V^1_0(\Xi)^4$ admits the asymptotic form

$$
\widehat{W}_{(1)}(\xi) = (M_{(1)} D(\nabla_\xi)\Phi_{(0)}(\xi)^\top)^\top + \widetilde{W}_{(1)}(\xi) \ , \tag{169}
$$

where the remainder $\widetilde{W}_{(1)}$ is subject to the estimates (55) with the majorants $c_k\rho^{-3-k+\delta}$ ($\delta > 0$ is arbitrary) and the notation used for the derivatives of the fundamental matrix $\Phi_{(0)}$ is matched with formulae (160) and (166).

In order to evaluate the correction term $M_{(1)}$ in the expansion of the polarization matrix the method [26] is employed, here we recall that the columns of the matrix

$$
\mathcal{W}_{(0)(-)}(\xi) = D_{(-)}(\xi)^\top + W_{(0)(-)}(\xi) \tag{170}
$$

(cf. (64)) are formal solutions to the homogeneous problem (168). By the Green formula in $\Xi \cap \mathbb{B}_R$, we obtain

(171)
$$\int_{\Xi\cap\mathbb{B}_R} \mathcal{W}_{(0)(-)}(\xi)^\top \widetilde{F}_{(1)}(\xi)d\xi + \int_{\partial\omega} \mathcal{W}_{(0)(-)}(\xi)^\top \widetilde{G}_{(1)}(\xi)ds_\xi =$$
$$\int_{\partial\mathbb{B}_R} (\widehat{W}_{(1)}(\xi)^\top D(|\xi|^{-1}\xi)^\top A^0_{(0)(-)} D(\xi)\mathcal{W}_{(0)(-)} - \mathcal{W}^\top_{(0)(-)} D(|\xi|^{-1}\xi)^\top A^0_{(0)(-)} D(\xi)\widehat{W}_{(1)}(\xi))ds_\xi$$
$$+O(R^{-1}) = -M_{(1)(=)} + O(R^{-1}) \,.$$

We have here repeated the computation (68) based on the representations (169) and (170). The integrand on the left-hand side of (171) is of order $|\xi|^{-4}$ and, hence, the integral over Ξ converges and the formula

(172)
$$M_{(1)(=)} = -\int_{\Xi} \mathcal{W}_{(0)(-)}(\xi)^\top \widetilde{F}_{(1)}(\xi)d\xi + \int_{\partial\omega} \mathcal{W}_{(0)(-)}(\xi)^\top \widetilde{G}_{(1)}(\xi)ds_\xi$$

together with (165)- (168) expresses the matrix $M_{(1)}$ (cf. the definition (63)) in terms of the matrix $A^{\mathsf{ME}} = (A^{\mathsf{EM}})^{-1}$ and the special solutions $W^1, \ldots, W^6$ and W^7, W^8, W^9 of the pure elasticity and the pure electricity exterior problems in Ξ. Theorem 3.4 shows that $(M^{\mathsf{ME}}_{(1)})^\top = -M^{\mathsf{EM}}_{(1)}$.

The formulae derived above can be used, e.g., to obtain the topological derivative of the electric enthalpy (136):

(173)
$$\mathcal{T}_{\mathcal{E}}(u;\omega) =$$
$$= \frac{1}{2}h^3((D^{\mathsf{M}}(\nabla_x)u^{\mathsf{M}}_{(0)}(0))^\top M^{\mathsf{M}} D^{\mathsf{M}}(\nabla_x)u^{\mathsf{M}}_{(0)}(0) - \nabla_x u^{\mathsf{E}}_{(0)}(0))^\top M^{\mathsf{E}} \nabla_x u^{\mathsf{E}}_{(0)}(0)))+$$
$$+h^3((D^{\mathsf{M}}(\nabla_x)u^{\mathsf{M}}_{(0)}(0))^\top M^{\mathsf{M}} D^{\mathsf{M}}(\nabla_x)u^{\mathsf{M}}_{(1)}(0) - \nabla_x u^{\mathsf{E}}_{(0)}(0))^\top M^{\mathsf{E}} \nabla_x u^{\mathsf{E}}_{(1)}(0)))+$$
$$+h^3\nabla_x u^{\mathsf{E}}_{(0)}(0))^\top M^{\mathsf{EM}} D^{\mathsf{M}}(\nabla_x)u^{\mathsf{M}}_{(1)}(0) + \ldots$$

Even the main term (with the factor $\frac{1}{2}h^3$) of the topological derivative (173) has no sign, that is, in contrast to the forms of topological derivatives of the energy functionals for the pure elasticity and the pure electricity problems. The correction term (with factor h^3) in (173) depends on two specific ingredients, namely, the correction term M^{EM} in polarization matrix (see (157) and (172)), and the correction terms $u^{\mathsf{M}}_{(1)}, u^{\mathsf{E}}_{(1)}$ for the combined mechanical and electric fields.

Remark 4.7. *All the attributes in the above formulae can be given explicitly for some canonical shapes, including balls, ellipsoids and elliptic cracks in three spatial dimensions, and some other shapes in two spatial dimensions (see* [44] *and* [49, 28, 23, 3] *and others).*

Remark 4.8. *The case of* $g^{\mathsf{E}} = 0$, $f^{\mathsf{E}} = 0$ *has a very clear physical meaning (i.e. one gets an electric sparkle when pressing the lighter button). Then, in notation of Section 4.2,*

$$\mathfrak{u}^{\mathsf{M}} = u, \quad \mathfrak{u}^{\mathsf{E}} = 0, \quad \mathfrak{e}^{\mathsf{M}} = \varepsilon^0, \quad \mathfrak{e}^{\mathsf{E}} = 0,$$

thus, by relation (63)*, we can conclude that the topological derivatives in* (63) *and* (69) *of the energy and electric enthalpy functionals coincides one with another. In general, this identity is false, and can be misleading for the choice of governing Gibbs' functional for piezoelectric body (cf. Remark 4.4). The relations between the topological derivatives for elasticity and piezoelectricity are easy to established, since the topological derivative for piezoelectricity can be viewed as the difference of that for elasticity and of the other for electricity.*

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