

# Shape Derivatives in Differential Forms II: Shape Derivatives for Scattering Problems

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# SHAPE DERIVATIVES IN DIFFERENTIAL FORMS II : SHAPE DERIVATIVES FOR SCATTERING PROBLEMS

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**Abstract.** In this paper we study shape derivatives of solutions of acoustic and electromagnetic scattering problems in frequency domain from the perspective of differential forms following [Ralf Hiptmair and Jingzhi Li, *Shape derivatives in differential forms I: an intrinsic perspective*, *Annali di Matematica Pura ed Applicata*, 192 (2013), pp. 1077–1098]. Relying on variational formulations, we present a unified framework for the derivation of strong and weak forms of derivatives with respect to variations of the shape of an impenetrable (resp. penetrable) scatterer, when we impose Dirichlet, Neumann, or impedance (resp. transmission) conditions on its boundary (resp. interface). In 3D for degrees  $l = 0$  and  $l = 1$  of the forms we obtain known and new formulas for shape derivatives of solutions of Helmholtz and Maxwell equations. They can form the foundation for numerical approximation with finite elements or boundary elements.

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**1. Introduction.** We consider the scattering of time-harmonic incident waves at a scatterer occupying the connected bounded domain  $\Omega \subset \mathbb{R}^d$ ,  $d \geq 2$ , with smooth boundary  $\Gamma = \partial\Omega$  of class  $C^3$ . Generically, linear homogeneous materials are assumed both in  $\Omega$  and  $\mathbb{R}^d \setminus \bar{\Omega}$ , but the scatterer can also be impenetrable. We aim for characterizations of the shape derivatives of weak solutions  $\omega$  with respect to variations of  $\Omega$ . To this end we have to select variational formulations that meet certain requirements. To understand these requirements let us first recall the concept of shape derivatives of functions and examine some of their properties.

**1.1. Shape derivative.** Clearly, the scattering solution  $\omega$  will depend on the shape of the scatterer  $\Omega$ . Since we can expect this dependence to be smooth, we can ask what is its derivative with respect to variations of  $\Omega$ , the *shape derivative*. Our approach to shape differentiability will be based on the velocity method (cf. [7,35]). First, we embed  $\Omega$  into a bounded “hold-all domain”  $\Omega_R$  with  $\Gamma_R = \partial\Omega_R$ , for instance a ball with sufficiently large fixed radius such that  $\Omega \Subset \Omega_R$ . Then, we pick a compactly supported velocity field  $\mathbf{v} \in C_0^2(\Omega_R)$ . Section 3.2 will give the rationale for the smoothness requirements on  $\mathbf{v}$ .

The velocity field  $\mathbf{v}$  induces a *flow*  $\mathbf{x} = \mathbf{x}(t, X)$  as solution of the family of initial value problems

$$\frac{\partial \mathbf{x}}{\partial t}(t, X) = \mathbf{v}(\mathbf{x}(t, X)), \quad \mathbf{x}(0, X) = X, \quad X \in \Omega_R. \quad (1.1)$$

A unique solution of the initial value problem (1.1) exists for all  $t \in \mathbb{R}$  and all  $X \in \Omega_R$ . Thus we can define a one-parameter group of  $C^2$ -diffeomorphisms  $T_t : \Omega_R \rightarrow \Omega_R$

$$T_t(\mathbf{v})X := \mathbf{x}(t, X), \quad t \in \mathbb{R}, X \in \Omega_R. \quad (1.2)$$

This generates a family of deformed domains

$$\Omega_t(\mathbf{v}) := T_t(\mathbf{v})(\Omega) = \{T_t(\mathbf{v})(X) : X \in \Omega\}. \quad (1.3)$$

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parametrized by *pseudo-time*  $t$ . Sometimes we drop  $\mathbf{v}$  and simply write  $T_t$  and  $\Omega_t$  when  $\mathbf{v}$  is inferred from the context. Since  $T_t$  is a diffeomorphism of class  $C^2$ , we see that the unit normal field  $\mathbf{n} = \mathbf{n}(t)$  on the boundary  $\Gamma_t := \partial(\Omega_t(\mathbf{v}))$  belongs to  $C^1(\Gamma_t, \mathbb{R}^d)$  [35, p. 16].

The set of admissible domains  $\mathcal{A}(\Omega_R)$  comprises smooth perturbations of  $\Omega$  and is formally given by

$$\mathcal{A}(\Omega_R) := \{T_t(\mathbf{v})(\Omega) : -1 < t < 1, \mathbf{v} \in C_0^2(\Omega_R, \mathbb{R}^d), \|\mathbf{v}\|_{C^2} < 1\}. \quad (1.4)$$

We write  $X(\wedge^l, \Omega_R)$  for a normed vector space of differential  $l$ -forms on  $\Omega_R$ , which is invariant under all *pullbacks*  $T_t(\mathbf{v})^*$  induced by the diffeomorphisms  $T_t(\mathbf{v})$ ,  $-1 < t < 1$ ,  $\mathbf{v} \in C_0^2(\Omega_R, \mathbb{R}^d)$ . By a shape-dependent differential form we mean a mapping  $\omega : \mathcal{A}(\Omega_R) \rightarrow X(\wedge^l, \Omega_R)$ .

DEFINITION 1.1 (Material derivative of a shape dependent differential form). (cf. [7, 35]) *Given a velocity field  $\mathbf{v} \in C_0^2(\Omega_R, \mathbb{R}^d)$ , a shape-dependent differential form  $\omega = \omega(\Omega)$  is said to have a material derivative at  $\Omega$  in the direction  $\mathbf{v}$  in  $X(\wedge^l, \Omega_R)$ , if the following limit exists in  $X(\wedge^l, \Omega_R)$*

$$\left\langle \frac{D\omega}{D\Omega}(\Omega), \mathbf{v} \right\rangle := \lim_{t \rightarrow 0^+} \frac{T_t(\mathbf{v})^* \omega(\Omega_t) - \omega(\Omega)}{t}, \quad (1.5)$$

and if the map  $\mathbf{v} \mapsto \left\langle \frac{D\omega}{D\Omega}(\Omega), \mathbf{v} \right\rangle \in X(\wedge^l, \Omega_R)$  is linear and continuous on  $C_0^2(\Omega_R, \mathbb{R}^d)$ .

Obviously, the material derivative is a Lagrangian concept. Also note that the material derivative may not vanish even for  $\mathbf{v}$  such that  $T_t(\mathbf{v})(\Omega) = \Omega$ . To factor out the impact of shape preserving transformations, we have to subtract a convective correction. This will involve the *Lie derivative* operator  $\mathcal{L}_{\mathbf{v}}$  [8, 9], which, in the calculus of differential forms, is the principal tool to take into account transport by a velocity field  $\mathbf{v}$ , cf. [20].

DEFINITION 1.2 (Shape derivative/domain derivative of a differential form). *We assume the same setting as in Definition 1.1. For an  $l$ -form  $\omega$  depending on the domain  $\Omega_t(\mathbf{v})$  its shape derivative/domain derivative at  $\Omega$  in the direction  $\mathbf{v} \in C^m(\Omega_R, \mathbb{R}^d)$  is*

$$\left\langle \frac{d\omega}{d\Omega}(\Omega), \mathbf{v} \right\rangle := \left\langle \frac{D\omega}{D\Omega}(\Omega), \mathbf{v} \right\rangle - \mathcal{L}_{\mathbf{v}}\omega(\Omega). \quad (1.6)$$

The specialization of this formula to functions, that is, the case  $l = 0$ , is already given in [35, Section 2.30].

As a shorthand notation for the shape derivative, we will also use  $\langle \delta\omega, \mathbf{v} \rangle$ , or simply  $\delta\omega$  when  $\mathbf{v}$  and  $\Omega$  are clear from the context. The shape derivative is a Eulerian concept, which is clear from an alternative definition in the sense of distributions:

$$\left\langle \frac{d\omega}{d\Omega}(\Omega), \mathbf{v} \right\rangle := \lim_{t \rightarrow 0^+} \frac{\omega(\Omega_t) - \omega(\Omega)}{t} \quad \text{in } \mathcal{D}'(\Omega_R, \wedge^l(\mathbb{R}^d)), \quad (1.7)$$

where  $\mathcal{D}'(\Omega_R, \wedge^l(\mathbb{R}^d))$  is the space of smooth compactly supported “test  $l$ -forms” on  $\Omega_R$ .

**1.2. Loss of smoothness for shape derivative: An example.** By Cartan’s formula  $\mathcal{L}_{\mathbf{v}} = i_{\mathbf{v}} \circ \mathbf{d} + \mathbf{d} \circ i_{\mathbf{v}}$ , where  $\mathbf{d}$  is the exterior derivative operator and  $i_{\mathbf{v}}$  stands for the contraction with some vector field  $\mathbf{v}$  [8]. Obviously, the Lie derivative involves exterior differentiation. Thus  $\mathcal{L}_{\mathbf{v}}\omega$  will incur a loss of smoothness compared to  $\omega$ . This will be inherited by the shape derivative and has prevented us from taking the limit (1.7) in the space  $X(\wedge^l, \Omega_R)$  where  $\omega$  lives:  $\left\langle \frac{d\omega}{d\Omega}(\Omega), \mathbf{v} \right\rangle \in X(\wedge^l, \Omega_R)$  cannot be expected, if  $X(\wedge^l, \Omega_R)$  is a space of differential forms characterized by smoothness requirements.

The following simple example for  $d = 1$  and functions (corresponding to 0-forms) strikingly illustrates this fact. We choose  $\Omega_R = ]-1, 1[$ , and the velocity field  $v(x) = 1 - x^2$ . The related family of flow diffeomorphisms is

$$T_t(x) = \tanh(t + \tanh^{-1}(x)), \quad -1 < x < 1.$$

Let  $\omega(\Omega)(x) = |x - s|$ ,  $-1 \leq s \leq 1$ , where  $s$  is the position of the interface  $\Gamma = \{s\}$  defining  $\Omega := ]s, 1[$ . Thus the dependence of  $\omega$  on  $s$  encodes the shape-dependence of the function  $x \mapsto \omega(\Omega)(x)$  in this particular setting. We compute the shape derivative at  $\Omega = ]0, 1[$ , that is, for  $s = 0$ . By straightforward calculations we can evaluate (1.7), and get

$$\frac{d\omega}{d\Omega}(\Omega)(x) = \left( \frac{d}{dt} |x - T_t(0)| \right)_{|_{t=0}} = \left( \frac{d}{dt} |x - \tanh(t)| \right)_{|_{t=0}} = \begin{cases} -1, & 0 \leq x < 1, \\ 1, & -1 < x < 0. \end{cases}$$

The loss of smoothness is obvious: although  $\omega(\Omega) \in H^1(]-1, 1[)$ , we have found  $\frac{d\omega}{d\Omega}(\Omega) \notin H^1(]-1, 1[)$ , but merely  $\frac{d\omega}{d\Omega}(\Omega) \in L^2(]-1, 1[)$ .

We can also apply Definition 1.2 to this example. We start with

$$\begin{aligned} (T_t(\mathbf{v})^* \omega(\Omega_t))(x) &= |T_t(x) - T_t(0)| = |\tanh(t + \tanh^{-1}(x)) - \tanh(t)| \\ &= \begin{cases} \tanh(t + \tanh^{-1}(x)) - \tanh(t) & \text{for } 0 \leq x < 1, \\ -\tanh(t + \tanh^{-1}(x)) + \tanh(t) & \text{for } -1 < x < 0. \end{cases} \end{aligned}$$

From  $\tanh' = 1 - \tanh^2$  it is immediate that

$$\frac{D\omega}{D\Omega}(\Omega) = \left( \frac{d}{dt} T_t(\mathbf{v})^* \omega(\Omega_t) \right)_{|_{t=0}} = \{x \mapsto -x|x|\}, \quad (1.8)$$

and

$$\mathcal{L}_{\mathbf{v}}\omega(x) = v(x) \frac{d\omega}{dx}(x) = \begin{cases} -v(x) = 1 - x^2, & 0 \leq x < 1, \\ v(x) = x^2 - 1, & -1 < x < 0. \end{cases}.$$

This complies with the above assertion that (1.6) and (1.7) agree. Indeed we have

$$\mathcal{L}_{\mathbf{v}}\omega(x) + \frac{d\omega}{d\Omega}(\Omega)(x) = \begin{cases} -x^2, & 0 \leq x < 1, \\ x^2, & -1 < x < 0 \end{cases} \quad \left[ = \frac{D\omega}{D\Omega}(\Omega)(x) \right].$$

We have highlighted the loss of smoothness, because we intend to characterize the shape derivatives  $\langle \delta\omega, \mathbf{v} \rangle$  as solutions of variational problems. As a consequence of the reduced smoothness of  $\langle \delta\omega, \mathbf{v} \rangle$  compared to  $\omega$  only variational formulations that make sense for non-smooth forms are eligible. It is important to keep this in mind to appreciate some of the considerations below.

**2. Related work, novelty, and outline.** This article supplements and extends our earlier work [20] that presented the first discussion of shape gradients and shape derivatives in the framework of exterior calculus of differential forms. As in [20] we emphasize that this perspective allows a unified and elegant treatment of a variety of second-order boundary value problems. In particular, our approach will cover acoustic and electromagnetic scattering. The power of exterior calculus has long been recognized in mathematical modelling and analysis of partial differential equations [8, 9], and, more recently, also in numerical analysis [1, 2, 19]. Yet, its use in shape calculus seems to be confined to [20].

As highlighted in the Introduction, shape calculus studies the impact of shape perturbations on shape dependent functions. During the last two decades it has been developed for scattering problems in acoustics and in electromagnetics, see [5, 6, 10, 13–16, 21, 22, 24, 26, 28, 29, 32–34]. In acoustic scattering problems, there are two general approaches to characterize shape derivatives, namely the *variational approach* and *boundary integral equation (BIE) method*. Results for sound-soft acoustic scattering were first obtained by Kirsch in [24] based on a variational formulation. Later this was generalized by Hettlich in [14, 15] for impedance and transmission conditions. In the BIE approach one differentiates boundary integral operators. This was applied to sound-soft and sound-hard scattering by Potthast in [32, 34], see also [21, 28]. The impedance case was later settled by Haddar and Kress in [10] based on [28]. The transmission case was successfully tackled by Hohage and Schormann [22] in two dimensions.

For electromagnetic (EM) scattering problems all theoretical results about shape derivatives were first derived through BIE methods. Consequently, all these results hold only for (piecewise) homogeneous media. EM obstacle scattering with perfect electric conductor (PEC) boundary conditions was addressed by Potthast in [33] via the BIE method and was also studied by Kress [27]. The EM obstacle scattering problem with impedance boundary conditions was investigated by Haddar and Kress in [10]. Quite recently, the electromagnetic transmission problem (medium scattering case) was successfully solved by Costabel and Le Louër [4] via the BIE method, for media with discontinuity only in the magnetic permeability. The essential difficulties in the variational approach are mainly due to the highly non-trivial shape-transformation of *curl*-related bilinear forms and boundary integrals involving tangential trace terms of electromagnetic fields, see the recent work of Hettlich [16].

The starting point for our investigations was the question “Can one derive, in the variational approach, a structural characterization of shape derivatives of solutions of electromagnetic scattering problems in the same fashion as for their acoustic counterparts?” What compounds difficulties for the standard approach are the complicated vector analytic expressions spawned by the domain perturbation. They also obscure the connection with the formulas derived for acoustic scattering.

By interpreting acoustic pressure as 0-form and electric and magnetic fields as 1-forms, and formulating abstract scattering problems in terms of differential forms, we observe that both problems belong to a single family of boundary value problems. Then we apply the structure theorems developed in [20] and, thus, we can give a unified characterization of the shape derivatives of solutions of scattering problems for all possible boundary (transmission) conditions for electromagnetics as well as acoustics in the language of differential forms.

The new theoretical contributions of this article are

1. a unified variational approach to treat scattering problems in the language of differential forms;
2. an explicit formula for the Dirichlet boundary conditions for the shape derivative of the electric field in electromagnetic obstacle scattering problems with PEC conditions;
3. a two-field variational formulation of transmission problems accommodating jumps across the interface;
4. a structure characterization of the shape derivative for electromagnetic transmission problems with discontinuity in both electric permittivity and magnetic permeability.

Moreover, our abstract theoretical results shed light on the structural similarity of shape derivatives in acoustic and electromagnetic scattering problems.

In the next section we are going to state scattering problems in the language of exterior calculus and introduce weak formulations in Sobolev spaces of differential forms. For trans-

mission problems we have to ensure that the variational problem can accommodate the scant smoothness of shape derivatives. The core part of this article is Section 4, where we establish boundary value problems or transmission problems, respectively – both in weak and strong form –, whose solutions yield the shape derivatives. Finally, in Section 5 we translate the general formulas into the language of vector calculus for  $l = 0$  (acoustic scattering) and  $l = 1$  (Maxwell's equations).

**3. Scattering problems.** As already stated, the scatterer occupies some interior domain  $\Omega \Subset \Omega_R$  with boundary  $\Gamma = \partial\Omega$ , and we denote the exterior domain  $\Omega^e = \Omega_R \setminus \overline{\Omega}$ . In this work, we shall state the abstract scattering problems in terms of differential forms, which covers both acoustic and electromagnetic scattering. The unknown total field will be denoted by an  $l$ -form  $\omega$  ( $l = 0$  for acoustics and  $l = 1$  for electromagnetics in  $\mathbb{R}^3$ ) with possible subscripts indicating interior and exterior domains. Readers are assumed to be familiar with exterior calculus and may refer to [8, 19, 20] for related notions and concepts. At the truncation boundary  $\Gamma_R$  we introduce (exact or approximate) absorbing boundary conditions in the form  $ABC(\omega) = g$ , where  $ABC$  is a linear operator on a suitable space of  $l$ -forms on  $\Omega^e$  and  $g$  stands for an excitation due to an incident field. Ideally,  $ABC(\omega)$  represents the exterior DtN map on  $\Omega_R$ . Since  $\Gamma_R$  will not be subject to deformation, details of  $ABC$  are not important for our considerations.

### 3.1. Scattering problems in strong form.

**3.1.1. Boundary value problems.** With  $\alpha, \kappa$  being smooth Riemannian metrics on  $\Omega_R$ , we write  $*_\alpha, *_\kappa$  for the associated Hodge operators

$$\begin{aligned} *_\alpha &: L^2(\Omega_R, \wedge^{l+1}(\mathbb{R}^d)) \mapsto L^2(\Omega_R, \wedge^{d-l-1}(\mathbb{R}^d)), \\ *_\kappa &: L^2(\Omega_R, \wedge^l(\mathbb{R}^d)) \mapsto L^2(\Omega_R, \wedge^{d-l}(\mathbb{R}^d)), \end{aligned}$$

which represent material properties. Here,  $L^2(\Omega_R, \wedge^l(\mathbb{R}^d))$  is the space of square integrable  $l$ -forms on  $\Omega_R$ .

We consider the following abstract boundary value problems, cf. [18, Section 2]:

$$(-1)^{d-l} \mathbf{d}(*_\alpha \mathbf{d}\omega) - *_\kappa \omega = 0 \quad \text{in } \Omega^e, \quad (3.1a)$$

$$BC(\omega) = 0 \quad \text{on } \Gamma := \partial\Omega, \quad (3.1b)$$

$$ABC(\omega) = g \quad \text{on } \Gamma_R, \quad (3.1c)$$

for the unknown  $l$ -form  $\omega$  on  $\Omega^e$ . Here,  $BC(\omega)$  denotes the boundary condition on the surface  $\Gamma$  of the scatterer, which is defined as

$$BC(\omega) := \begin{cases} \text{Tr } \omega, & \text{Dirichlet case,} & (3.2a) \\ \text{Tr}(*_\alpha \mathbf{d}\omega), & \text{Neumann case,} & (3.2b) \\ \text{Tr}(*_\alpha \mathbf{d}\omega) + i(-1)^{d-l-1} *_\lambda^\Gamma(\text{Tr } \omega), & \text{impedance case,} & (3.2c) \end{cases}$$

where  $\text{Tr}$  designates the trace of differential forms onto  $\Gamma$  and  $i$  is the imaginary unit. Both, the absorbing boundary operator  $ABC$  and the impedance operator  $*_\lambda^\Gamma$  should match in order to guarantee the existence and uniqueness of solutions.

Since the boundary  $\Gamma$  will be subject to perturbations, an intrinsic Hodge operator  $*_\lambda^\Gamma$  on  $\Gamma$  seems problematic. Therefore, the following assumption is natural.

**ASSUMPTION 1 (Impedance metric).** *The Hodge operator  $*_\lambda^\Gamma$  is associated with a Riemannian metric on  $\Gamma$  that is the restriction of  $\lambda \cdot$  the Euclidean metric on  $\Omega_R$  to  $\Gamma$  for some  $\lambda > 0$ .*

In a sense, we regard  $*_{\lambda}^{\Gamma}$  as induced by the Euclidean volume Hodge operator  $*$  on  $\Omega_R$ : “ $*_{\lambda}^{\Gamma} = \lambda *_{|\Gamma}$ ”. Then, it can be verified by straightforward calculation (see Appendix A) that

$$*_{\lambda}^{\Gamma} \text{Tr}(\boldsymbol{\omega}) = \lambda \text{Tr}(i_{\mathbf{n}} * \boldsymbol{\omega}) \quad \text{for } \boldsymbol{\omega} \in C^0(\wedge^l(\overline{\Omega}_R)), \quad (3.3)$$

where  $\mathbf{n} : \Gamma \rightarrow \mathbb{R}^d$  is the (Euclidean) exterior unit vector field on  $\Gamma$ . We keep the same notation for a  $C^1$ -extension of  $\mathbf{n}$  to a tubular neighborhood of  $\Gamma$ . Thanks to (3.3), under Assumption 1 the impedance boundary condition (3.2c) can be rewritten as

$$BC(\boldsymbol{\omega}) = \text{Tr}(*_{\alpha} \mathbf{d} \boldsymbol{\omega}) + i(-1)^{d-l-1} \lambda \text{Tr}(i_{\mathbf{n}} * \boldsymbol{\omega}) = 0 \quad \text{on } \Gamma. \quad (3.4)$$

We observe that, using (3.1a), the boundary condition (3.2c) implies for the solution of (3.1)

$$\text{Tr}(*_{\kappa} \boldsymbol{\omega}) - i\lambda \text{Tr}(\mathbf{d}(i_{\mathbf{n}} * \boldsymbol{\omega})) = 0 \quad \text{on } \Gamma, \quad (3.5)$$

because the exterior derivative commutes with the trace operator.

**3.1.2. Transmission problems.** Assume that besides  $\alpha$  and  $\kappa$ , we are given another pair of “interior” smooth Riemannian metrics  $\alpha_i, \kappa_i$  on  $\Omega_R$ , inducing Hodge operators

$$\begin{aligned} *_{\alpha_i} &: \mathbf{L}^2(\Omega_R, \wedge^{l+1}(\mathbb{R}^d)) \mapsto \mathbf{L}^2(\Omega_R, \wedge^{d-l-1}(\mathbb{R}^d)), \\ *_{\kappa_i} &: \mathbf{L}^2(\Omega_R, \wedge^l(\mathbb{R}^d)) \mapsto \mathbf{L}^2(\Omega_R, \wedge^{d-l}(\mathbb{R}^d)). \end{aligned}$$

Then we can state the abstract transmission problems as follows:

$$(-1)^{d-l} \mathbf{d}(*_{\alpha_i} \mathbf{d} \boldsymbol{\omega}^i) - *_{\kappa_i} \boldsymbol{\omega}^i = 0 \quad \text{in } \Omega, \quad (3.6a)$$

$$(-1)^{d-l} \mathbf{d}(*_{\alpha_e} \mathbf{d} \boldsymbol{\omega}^e) - *_{\kappa_e} \boldsymbol{\omega}^e = 0 \quad \text{in } \Omega^e, \quad (3.6b)$$

$$IC(\boldsymbol{\omega}) = 0 \quad \text{on } \Gamma, \quad (3.6c)$$

$$ABC(\boldsymbol{\omega}) = g \quad \text{on } \Gamma_R, \quad (3.6d)$$

where  $\alpha_e = \alpha, \kappa_e = \kappa$  in  $\Omega^e$ . We set  $\boldsymbol{\omega} := \boldsymbol{\omega}^i$  in  $\Omega$  and  $\boldsymbol{\omega} := \boldsymbol{\omega}^e$  in  $\Omega^e$ . Then the general interface transmission condition  $IC(\boldsymbol{\omega})$  can be expressed as

$$IC(\boldsymbol{\omega}) = \begin{cases} [\text{Tr } \boldsymbol{\omega}]_{\Gamma} & \text{(Dirichlet jump),} \\ [\text{Tr}(*_{\alpha} \mathbf{d} \boldsymbol{\omega})]_{\Gamma} & \text{(Neumann jump),} \end{cases} \quad (3.7)$$

with jump operators defined according to

$$\begin{aligned} [\text{Tr } \boldsymbol{\omega}]_{\Gamma}(\mathbf{x}) &:= \text{Tr} \left( \lim_{\Omega \ni \mathbf{z}^i \rightarrow \mathbf{x}} \boldsymbol{\omega}^i(\mathbf{z}^i) - \lim_{\Omega^e \ni \mathbf{z}^e \rightarrow \mathbf{x}} \boldsymbol{\omega}^e(\mathbf{z}^e) \right), \\ [\text{Tr}(*_{\alpha} \mathbf{d} \boldsymbol{\omega})]_{\Gamma}(\mathbf{x}) &:= \text{Tr} \left( \lim_{\Omega \ni \mathbf{z}^i \rightarrow \mathbf{x}} *_{\alpha_i} \mathbf{d} \boldsymbol{\omega}^i(\mathbf{z}^i) - \lim_{\Omega^e \ni \mathbf{z}^e \rightarrow \mathbf{x}} *_{\alpha_e} \mathbf{d} \boldsymbol{\omega}^e(\mathbf{z}^e) \right), \end{aligned} \quad \mathbf{x} \in \Gamma, \quad (3.8)$$

where the limits are supposed to be well defined.

**3.2. Regularity.** The smoothness of  $\partial\Omega$  and of the coefficient metrics can be expected to induce smoothness of solutions of boundary value problems and transmission problems. In the framework of exterior calculus, we rely on the following Sobolev spaces of differential forms on a generic smooth domain  $D \subset \mathbb{R}^d$  to characterize smoothness

$$\mathbf{H}^k(\mathbf{d}, D, \wedge^l(\mathbb{R}^d)) := \left\{ \boldsymbol{\omega} \in \mathbf{H}^k(D; \wedge^l(\mathbb{R}^d)) \mid \mathbf{d} \boldsymbol{\omega} \in \mathbf{H}^k(D; \wedge^{l+1}(\mathbb{R}^d)) \right\}, \quad (3.9)$$

for  $k \in \mathbb{N} \cup \{0\}$  with the natural graph norms

$$\|\omega\|_{\mathbf{H}^k(\mathbf{d}, D, \wedge^l(\mathbb{R}^d))}^2 := \|\omega\|_{\mathbf{H}^k(D, \wedge^l(\mathbb{R}^d))}^2 + \|\mathbf{d}\omega\|_{\mathbf{H}^k(D, \wedge^{l+1}(\mathbb{R}^d))}^2, \quad (3.10)$$

In the case  $k = 0$  we simply write  $\mathbf{H}(\mathbf{d}, D, \wedge^l(\mathbb{R}^d)) := \mathbf{H}^0(\mathbf{d}, D, \wedge^l(\mathbb{R}^d))$  and  $\mathbf{H}^0(D, \wedge^l(\mathbb{R}^d)) := \mathbf{L}^2(D, \wedge^l(\mathbb{R}^d))$ . We remind that in terms of vector proxies in  $\mathbb{R}^3$   $\mathbf{H}(\mathbf{d}, D, \wedge^l(\mathbb{R}^d))$  corresponds to the Sobolev spaces  $H^1(D)$ ,  $\mathbf{H}(\mathbf{curl}; D)$ ,  $\mathbf{H}(\mathbf{div}; D)$  when  $l = 0, 1, 2$  in  $\mathbb{R}^3$ , respectively. We refer readers to [20, Sect. 2] for more details and further references.

Unfortunately, a general elliptic regularity theory in the framework of differential forms in arbitrary dimensions does not seem to be available. Therefore, we make the following plausible assumption.

**ASSUMPTION 2.** *Both (3.1) and (3.6) are supposed to have unique solutions  $\omega$  that satisfy*

- (i)  $\omega \in \mathbf{H}^1(\mathbf{d}, \Omega^e, \wedge^l(\mathbb{R}^d))$  for the boundary value problem (3.1),
- (ii)  $\omega \in \mathbf{H}^1(\mathbf{d}, \Omega_R \setminus \Gamma, \wedge^l(\mathbb{R}^d))$  for the transmission problem (3.6),

respectively.

Such results are well known for  $d = 2, 3$  and the scalar case  $l = 0$ , see [30, Chapter 4]. Also for  $d = 3$  and  $l = 1$ , that is for Maxwell's equations in frequency domain, Assumption 2 has been confirmed, see [3].

Thanks to the smoothness of the deformation velocity field  $\mathbf{v} \in C_0^2(\Omega_R, \mathbb{R}^d)$ , the regularity assumption above will also carry over to the material derivatives  $\langle \frac{D\omega}{D\Omega}(\Omega), \mathbf{v} \rangle$ . Conversely, taking Lie derivatives of the solutions  $\omega$  loses one order of differentiability, which means

$$\mathcal{L}_{\mathbf{v}}\omega \in \begin{cases} \mathbf{H}(\mathbf{d}, \Omega^e, \wedge^l(\mathbb{R}^d)) & \text{for the boundary value problem (3.1),} \\ \mathbf{H}(\mathbf{d}, \Omega_R \setminus \Gamma, \wedge^l(\mathbb{R}^d)) & \text{for the transmission problem (3.6).} \end{cases} \quad (3.11)$$

Therefore, in the case of the transmission problem (3.6), though the solution belongs to  $\mathbf{H}(\mathbf{d}, \Omega_R, \wedge^l(\mathbb{R}^d))$ , its shape derivative according to Definition 1.2 will usually merely possess the low regularity (3.11) of the Lie derivative: f

**COROLLARY 3.1.** *Under Assumption 2 and for  $\mathbf{v} \in C_0^2(\Omega_R, \mathbb{R}^d)$  the shape derivatives  $\langle \delta\omega, \mathbf{v} \rangle$  of solutions  $\omega$  of the boundary value problem and transmission problem presented above will satisfy*

$$\langle \delta\omega, \mathbf{v} \rangle \in \begin{cases} \mathbf{H}(\mathbf{d}, \Omega^e, \wedge^l(\mathbb{R}^d)) & \text{for the boundary value problem (3.1),} \\ \mathbf{H}(\mathbf{d}, \Omega_R \setminus \Gamma, \wedge^l(\mathbb{R}^d)) & \text{for the transmission problem (3.6).} \end{cases} \quad (3.12)$$

**3.3. Variational formulations.** In order to state the boundary value problems and transmission problems in variational (weak) form, below we rely on the Hilbert spaces from (3.9) for  $k = 0$ , denoted by  $\mathbf{H}(\mathbf{d}, \Omega, \wedge^l(\mathbb{R}^d))$ . In addition, as in [16, Section 2] for the variational formulations we will assume that the absorbing boundary conditions  $ABC(\omega) = g$  on  $\Gamma_R$  are given in the more specific form of an (exact or approximate) DtN operator

$$\mathcal{T} : \text{Tr}(\mathbf{H}(\mathbf{d}, \Omega_R, \wedge^l(\mathbb{R}^d))) \mapsto \text{Tr}(\mathbf{H}(\mathbf{d}, \Omega_R, \wedge^{d-l-1}(\mathbb{R}^d))) \quad (3.13)$$

as

$$ABC(\omega) = g \iff \text{Tr}(*_{\alpha}\mathbf{d}\omega) = \mathcal{T}(\text{Tr}(\omega)) + g \quad \text{on } \Gamma_R, \quad (3.14)$$

where  $g$  is the trace of an incident field  $\in \mathbf{H}_{\text{loc}}^1(\mathbb{R}^d, \wedge^{d-l-1}(\mathbb{R}^d))$  onto  $\Gamma_R$ . Concrete incarnations of such DtN maps are known for both Helmholtz equation (cf. [24, p. 84]) and Maxwell systems (cf. [25, Lemmas 3.4 and 4.3]). In the following subsections we will present variational formulations of the boundary value/transmission problems (3.1) or (3.6).

**3.3.1. BVP with impedance and Neumann boundary conditions.** We will treat abstract obstacle scattering problems with impedance boundary conditions first. Note that impedance boundary conditions reduce to Neumann boundary conditions when  $*_{\lambda}^{\Gamma}$  vanishes.

For abstract obstacle scattering problems with impedance boundary condition, the variational formulation directly arises from integration by parts and reads: seek a differential form  $\omega \in V := \{\omega \in \mathbf{H}(\mathbf{d}, \Omega^e, \wedge^l(\mathbb{R}^d)), \text{Tr}(\omega) \in \mathbf{L}^2(\Gamma, \wedge^l(\Gamma))\}$  such that for all smooth test forms  $\eta \in \mathcal{DF}^{l,\infty}(\overline{\Omega}_R)$  the following holds true

$$\mathbf{a}_I(\omega, \eta) = (-1)^{d-l+1} \int_{\partial\Omega_R} g \wedge \text{Tr} \eta, \quad (3.15)$$

with a bilinear form

$$\begin{aligned} \mathbf{a}_I(\omega, \eta) := & \int_{\Omega^e} *_{\alpha} \mathbf{d} \omega \wedge \mathbf{d} \eta - *_{\kappa} \omega \wedge \eta + i \int_{\Gamma} *_{\lambda}^{\Gamma}(\text{Tr} \omega) \wedge \text{Tr} \eta - \\ & (-1)^{d-l} \int_{\partial\Omega_R} (\mathcal{I}(\text{Tr}(\omega))) \wedge \text{Tr} \eta. \end{aligned} \quad (3.16)$$

Above we opted for the test space  $\mathcal{DF}^{l,\infty}(\overline{\Omega}_R)$ . By density this is equivalent to testing with  $\eta \in V$ . For all variational problems presented in the sequel this argument holds true. Though we state them for test spaces of smooth forms, those can usually be replaced with those Sobolev spaces of forms used as trial spaces.

**3.3.2. BVP with Dirichlet BC.** In order to avoid imposing essential boundary conditions on trial and test functions, following [20] we switch to a dual (mixed) variational formulation. To derive the dual formulation, we introduce a  $(d-l-1)$ -form,

$$\rho = *_{\alpha} \mathbf{d} \omega \quad \Leftrightarrow *_{\alpha^{-1}} \rho = (-1)^{(l+1)(d-1)} \mathbf{d} \omega. \quad (3.17)$$

where  $\alpha^{-1}$  is the inverse of the metric  $\alpha$ , which means that  $*_{\alpha^{-1}} *_{\alpha} = (-1)^{(l+1)(d-1)} \text{Id}$ . Then the PDE (3.1a) can be rewritten as

$$(-1)^{d-l} \mathbf{d} \rho - *_{\kappa} \omega = 0 \quad \text{in } \Omega^e. \quad (3.18)$$

We test both (3.17) and (3.18) and apply integration by parts. Thanks to the homogeneous Dirichlet conditions boundary terms will vanish. This yields the dual saddle-point formulation: Seek  $\omega \in \mathbf{L}^2(\Omega^e, \wedge^l(\mathbb{R}^d))$  and  $\rho \in \mathbf{H}(\mathbf{d}, \Omega^e, \wedge^{d-l-1}(\mathbb{R}^d))$

$$\mathbf{a}_D \left( \begin{pmatrix} \rho \\ \omega \end{pmatrix}, \begin{pmatrix} \tau \\ \nu \end{pmatrix} \right) = (-1)^{(l+1)} \int_{\partial\Omega_R} g \wedge \text{Tr} \tau \quad (3.19)$$

for all smooth  $\tau \in \mathcal{DF}^{d-l-1,\infty}(\overline{\Omega}_R)$  and  $\nu \in \mathcal{DF}^{l,\infty}(\overline{\Omega}_R)$ , with

$$\begin{aligned} \mathbf{a}_D \left( \begin{pmatrix} \rho \\ \omega \end{pmatrix}, \begin{pmatrix} \tau \\ \nu \end{pmatrix} \right) := & \int_{\Omega_R \setminus \Omega} *_{\alpha^{-1}} \rho \wedge \tau + (-1)^{(l+1)d} \omega \wedge \mathbf{d} \tau + \\ & (-1)^{(l+1)} \int_{\partial\Omega_R} \mathcal{I}^{-1}(\text{Tr}(\rho)) \wedge \text{Tr} \tau + \\ & \int_{\Omega^e} (-1)^{(d-l)} \mathbf{d} \rho \wedge \nu - *_{\kappa} \omega \wedge \nu. \end{aligned} \quad (3.20)$$

**3.3.3. Transmission problems.** As pointed out in Section 1.2, for deriving shape derivatives it will be essential to use a variational formulation that does not require any continuity across the interface  $\Gamma$ . This is satisfied by the following *two-field variational formulation* in saddle-point form: Seek a pair of differential forms  $\omega^e \in \mathbf{H}(\mathbf{d}, \Omega_R, \wedge^l(\mathbb{R}^d))$  and  $\omega^i \in \mathbf{H}(\mathbf{d}, \Omega_R, \wedge^l(\mathbb{R}^d))$  such that for all smooth test forms  $\eta \in \mathcal{DF}^{l,\infty}(\overline{\Omega}_R)$ ,  $\mu \in \mathcal{DF}^{d-l-1,\infty}(\overline{\Omega}_R)$  (which are independent of  $\Omega$ )

$$\mathfrak{a}_T \left( \begin{pmatrix} \omega^e \\ \omega^i \end{pmatrix}, \begin{pmatrix} \eta \\ \mu \end{pmatrix} \right) = (-1)^{d-l} \int_{\Gamma_R} g \wedge \text{Tr } \eta^e, \quad (3.21)$$

with a bilinear form  $\mathfrak{a}_T$  defined as

$$\begin{aligned} \mathfrak{a}_T \left( \begin{pmatrix} \omega^e \\ \omega^i \end{pmatrix}, \begin{pmatrix} \eta \\ \mu \end{pmatrix} \right) := \\ \int_{\Omega^e} *_{\alpha_e} \mathbf{d} \omega^e \wedge \mathbf{d} \eta - \int_{\Omega^e} *_{\kappa_e} \omega^e \wedge \eta - (-1)^{d-l} \int_{\Gamma_R} \mathcal{F}(\text{Tr}(\omega^e)) \wedge \text{Tr } \eta + \\ \int_{\Omega} *_{\alpha_i} \mathbf{d} \omega^i \wedge \mathbf{d} \eta - \int_{\Omega} *_{\kappa_i} \omega^i \wedge \eta + \int_{\Gamma} [\text{Tr}(\omega)] \wedge \text{Tr } \mu \end{aligned} \quad (3.22)$$

The transmission conditions (3.6c) are implied by (3.21) as can be seen from integration by parts. From (3.21) we can recover the scattering solution as

$$\omega := \begin{cases} \omega^i & \text{in } \Omega \\ \omega^e & \text{in } \Omega^e \end{cases} \in \mathbf{H}(\mathbf{d}, \Omega_R \setminus \Gamma, \wedge^l(\mathbb{R}^d)). \quad (3.23)$$

**4. Shape derivatives for solutions of scattering problems.** Our policy is to arrive at variational characterizations of shape derivatives by implicit shape differentiation of variational equations. This entails computing the shape gradients of (bi-)linear forms.

**4.1. Existence of shape derivatives.** Thanks to Assumption 2, the existence of the shape derivatives  $\langle \delta \omega, \mathbf{v} \rangle$  according to Definition 1.2 for weak solutions of the various boundary value/transmission problem can be concluded from the existence of material derivatives. That is tackled by implicit differentiation of variational equations. We elaborate this for (3.15), which we now write as: seek  $\omega \in V$  such that for all  $\eta \in \mathcal{DF}^{l,\infty}(\overline{\Omega}_R)$

$$\int_{\Omega_t^e} *_{\alpha} \mathbf{d} \omega_t \wedge \mathbf{d} \eta - *_{\kappa} \omega_t \wedge \eta + i \int_{\Gamma_t} *_{\lambda}^{\Gamma} (\text{Tr } \omega_t) \wedge \text{Tr } \eta + ABC(\omega_t, \eta) = \ell(\eta).$$

Here, a subscript  $t$  indicates shape dependence on pseudo-time through the flow  $T_t(\mathbf{v})$  defined in (1.2). No such dependence affects both  $ABC(\cdot)$  and the right-hand side  $\ell(\cdot)$ . Pulling back to the reference configuration ( $t = 0$ ) we get

$$\begin{aligned} \int_{\Omega^e} T_t^* (*_{\alpha} \mathbf{d} \omega_t) \wedge T_t^* \eta - T_t^* (*_{\kappa} \omega_t) \wedge T_t^* \eta + i \int_{\Gamma} T_t^* (*_{\lambda}^{\Gamma} (\text{Tr } \omega_t)) \wedge \text{Tr}(T_t^* \eta) + \\ ABC(T_t^* \omega_t, \eta) = \ell(T_t^* \eta). \end{aligned} \quad (4.1)$$

Introduce  $M_{\alpha}(t) := T_t^* *_{\alpha} T_t^{-*}$ ,  $M_{\kappa}(t) := T_t^* *_{\kappa} T_t^{-*}$ , and  $M_{\lambda} := T_t^* *_{\lambda}^{\Gamma} T_t^{-*}$ , which are  $t$ -dependent linear operators that, for every  $\mathbf{x} \in \Omega_R / \mathbf{x} \in \Gamma$ , act on spaces of alternating multilinear forms. Owing to the smoothness of  $\mathbf{v}$  and of the metrics  $\alpha$ ,  $\kappa$ , and  $\lambda$ , these operators will be continuously differentiable w.r.t.  $t$ . Thus we can rewrite (4.1) as, with  $\hat{\eta} := T_t^* \eta$ ,

$$\int_{\Omega^e} M_\alpha(t)(\mathbf{d}T_t^*\boldsymbol{\omega}_t)\wedge\mathbf{d}\widehat{\boldsymbol{\eta}} - M_\kappa(t)(T_t^*\boldsymbol{\omega})\wedge T_t^*\boldsymbol{\eta} + \mathbf{i} \int_{\Gamma} M_\lambda(t)(\text{Tr}T_t^*\boldsymbol{\omega})\wedge\text{Tr}\widehat{\boldsymbol{\eta}} + ABC(T_t^*\boldsymbol{\omega}, \widehat{\boldsymbol{\eta}}) = \ell(\widehat{\boldsymbol{\eta}}). \quad (4.2)$$

We can assume the test form  $\widehat{\boldsymbol{\eta}}$  to be independent of  $t$ . Since  $M_\alpha(0) = *_\alpha$ ,  $M_\kappa(0) = *_\kappa$ , and  $M_\lambda(0) = *_\lambda^\Gamma$ , differentiation of (4.2) w.r.t  $t$  and evaluation at  $t = 0$  yields a variational equation for the material derivative

$$\int_{\Omega^e} *_\alpha \mathbf{d} \frac{D\boldsymbol{\omega}}{D\Omega}(\mathbf{v}) \wedge \mathbf{d}\boldsymbol{\eta} + \dot{M}_\alpha(0) \mathbf{d}\boldsymbol{\omega} \wedge \mathbf{d}\boldsymbol{\eta} - *_\kappa \frac{D\boldsymbol{\omega}}{D\Omega}(\mathbf{v}) \wedge \boldsymbol{\eta} - \dot{M}_\kappa(0) \boldsymbol{\omega} \wedge \boldsymbol{\eta} + \mathbf{i} \int_{\Gamma} *_\lambda^\Gamma(\text{Tr} \frac{D\boldsymbol{\omega}}{D\Omega}(\mathbf{v})) \wedge \text{Tr} \boldsymbol{\eta} + \dot{M}_\lambda(0) \text{Tr} \boldsymbol{\omega} \wedge \text{Tr} \boldsymbol{\eta} + ABC(\frac{D\boldsymbol{\omega}}{D\Omega}(\mathbf{v}), \boldsymbol{\eta}) = 0, \quad (4.3)$$

for all  $\boldsymbol{\eta} \in V := \{\boldsymbol{\omega} \in \mathbf{H}(\mathbf{d}, \Omega^e, \wedge^l(\mathbb{R}^d)), \text{Tr}(\boldsymbol{\omega}) \in \mathbf{L}^2(\Gamma, \wedge^l(\Gamma))\}$ . Hence, the material derivative  $\frac{D\boldsymbol{\omega}}{D\Omega}(\mathbf{v})$  is recovered as the unique solution  $\in V$  of an impedance boundary value problem. From their definition it is also immediate that the derivatives  $\dot{M}_\alpha(0)$ ,  $\dot{M}_\kappa(0)$ , and  $\dot{M}_\lambda(0)$  all depend linearly on  $\mathbf{v}$  (through the Jacobians  $D\mathbf{v}$ ) and are bounded as linear mappings on  $C_0^1(\Omega_R)$ . Summing up, (4.3) defines a linear mapping  $\mathbf{v} \mapsto \frac{D\boldsymbol{\omega}}{D\Omega}(\mathbf{v}) \in V$ , continuous on  $C_0^1(\Omega_R)$ .

**4.2. Shape gradients of integrals of forms.** Following [20, Section 3] we briefly review shape gradients for domain and boundary integrals. They play an important role in deriving formulas for shape derivatives, because our approach boils down to computing shape gradients of variational equations.

In the sequel we fix a  $C^2$ -domain  $\Omega \Subset \Omega_R$ . Motivated by the terms occurring in the bilinear forms  $\mathfrak{a}_I$ ,  $\mathfrak{a}_D$  and  $\mathfrak{a}_T$ , we consider the domain integral of a shape-dependent  $d$ -form, a density form  $D \mapsto \boldsymbol{\omega}(D) \in \mathbf{H}^1(\Omega_R; \wedge^d(\mathbb{R}^d))$ ,  $D \in \mathcal{A}(\Omega_R)$  as defined in (1.4):

$$J(D) = \int_D \boldsymbol{\omega}(D), \quad D \in \mathcal{A}(\Omega_R). \quad (4.4)$$

**LEMMA 4.1** (Shape gradient of volume integrals, see [20, Thm 3.4]). *Assume that  $\boldsymbol{\omega}(D) \in \mathbf{H}^1(\Omega_R; \wedge^d(\mathbb{R}^d))$  for all admissible domains  $D \in \mathcal{A}(\Omega_R)$  and that  $D \mapsto \boldsymbol{\omega}(D)$  is shape differentiable at  $\Omega$  with shape derivative  $\mathbf{v} \mapsto \langle \delta\boldsymbol{\omega}, \mathbf{v} \rangle \in \mathbf{H}^0(\Omega_R, \wedge^d(\mathbb{R}^d))$ .*

*Then the domain functional  $D \mapsto J(D)$  from (4.4) possesses a shape gradient at  $\Omega$  given by  $(\Omega_t(\mathbf{v}))$  as in (1.3))*

$$\langle dJ(\Omega), \mathbf{v} \rangle := \lim_{t \rightarrow 0^+} \frac{J(\Omega_t(\mathbf{v})) - J(\Omega)}{t} = \int_{\partial\Omega} \text{Tr}(i_{\mathbf{v}}\boldsymbol{\omega}) + \int_{\Omega} \langle \delta\boldsymbol{\omega}, \mathbf{v} \rangle. \quad (4.5)$$

*Proof.* We use the notations of Section 1.1 and for the sake of brevity we write  $\Omega_t := \Omega_t(\mathbf{v})$  and  $T_t := T_t(\mathbf{v})$ .

$$\begin{aligned} \lim_{t \rightarrow 0} \frac{1}{t} \left( \int_{\Omega_t} \boldsymbol{\omega}(\Omega_t) - \int_{\Omega} \boldsymbol{\omega}(\Omega) \right) &= \lim_{t \rightarrow 0} \frac{1}{t} \int_{\Omega} T_t^* \boldsymbol{\omega}(\Omega_t) - \boldsymbol{\omega}(\Omega) \\ &= \lim_{t \rightarrow 0} \frac{1}{t} \int_{\Omega} T_t^* \boldsymbol{\omega}(\Omega_t) - T_t^* \boldsymbol{\omega}(\Omega) + T_t^* \boldsymbol{\omega}(\Omega) - \boldsymbol{\omega}(\Omega) \\ &= \lim_{t \rightarrow 0} \int_{\Omega} T_t^* \frac{\boldsymbol{\omega}(\Omega_t) - \boldsymbol{\omega}(\Omega)}{t} + \lim_{t \rightarrow 0} \int_{\Omega} \frac{T_t^* \boldsymbol{\omega}(\Omega) - \boldsymbol{\omega}(\Omega)}{t} \\ &= \int_{\Omega} \langle \delta\boldsymbol{\omega}, \mathbf{v} \rangle + \int_{\Omega} \mathcal{L}_{\mathbf{v}} \boldsymbol{\omega}(\Omega) = \int_{\Omega} \langle \delta\boldsymbol{\omega}, \mathbf{v} \rangle + \int_{\partial\Omega} \text{Tr}(i_{\mathbf{v}}\boldsymbol{\omega}(\Omega)), \end{aligned}$$

by Stokes theorem, since  $\mathcal{L}_{\mathbf{v}}\omega = \mathbf{d}i_{\mathbf{v}}\omega$ . In addition we used  $\lim_{t \rightarrow 0} T_t^* = Id$ . The boundary term is well defined due to  $i_{\mathbf{v}}\omega(\Omega) \in \mathbf{H}^1(\Omega; \wedge^{d-1}(\mathbb{R}^d))$ . Linearity and continuity in  $\mathbf{v}$  is clear.  $\square$

We may also consider the boundary integral associated with a shape-dependent  $(d-1)$ -form  $\boldsymbol{\eta}(D) \in \mathbf{H}^1(\Omega_R; \wedge^{d-1}(\mathbb{R}^d))$ , for all admissible domains  $D \in \mathcal{A}(\Omega_R)$ , over  $\partial D$ , which is an oriented manifold without boundary in  $\mathbb{R}^d$  of codimension one,

$$I(D) = \int_{\partial D} \text{Tr} \boldsymbol{\eta} . \quad (4.6)$$

LEMMA 4.2 (Shape gradient of boundary integrals, see [20, Cor. 3.5]). *Assume that  $\boldsymbol{\eta}(D) \in \mathbf{H}^1(\Omega_R; \wedge^{d-1}(\mathbb{R}^d))$  for all admissible domains  $D \subset \Omega_R$  and that  $D \mapsto \boldsymbol{\eta}(D)$  is shape differentiable at  $\Omega$  with shape derivative  $\mathbf{v} \mapsto \langle \delta \boldsymbol{\eta}, \mathbf{v} \rangle \in \mathbf{H}^0(\Omega_R; \wedge^{d-1}(\mathbb{R}^d))$ .*

*Then the boundary integral  $D \mapsto I(D)$  from (4.6) is shape differentiable at  $\Omega$ , with shape gradient*

$$\langle dI(\Omega), \mathbf{v} \rangle := \lim_{t \rightarrow 0} \frac{I(\Omega_t(\mathbf{v})) - I(\Omega)}{t} = \int_{\partial \Omega} \text{Tr}(i_{\mathbf{v}} \mathbf{d} \boldsymbol{\eta}) + \int_{\partial \Omega} \langle \delta \boldsymbol{\eta}, \mathbf{v} \rangle . \quad (4.7)$$

*Proof.* By Stokes' theorem  $\int_{\partial \Omega} \boldsymbol{\eta} = \int_{\Omega} \mathbf{d} \boldsymbol{\eta}$  and the assertion is immediate from Lemma 4.1 and the fact that linear mappings commute with the shape derivative.  $\square$

Moreover, since bilinear forms are the main building blocks of variational forms of PDEs, we make explicit the shape derivative of abstract bilinear forms in the following lemma.

LEMMA 4.3 (Shape gradient of bilinear volume integral, see [20, Cor. 3.6]). *For two shape-dependent  $l$ -forms,  $\omega, \boldsymbol{\eta} \in \mathbf{H}^1(\mathbf{d}, \Omega_R, \wedge^l(\mathbb{R}^d))$  ( $0 \leq l \leq d-1$ ) that are shape-differentiable at  $\Omega$  the bilinear form given by*

$$\mathcal{B}(D) = \int_D * \mathbf{d} \omega \wedge \mathbf{d} \boldsymbol{\eta} , \quad D \in \mathcal{A}(\Omega_R) , \quad (4.8)$$

*has the following shape gradient at  $\Omega$*

$$\langle d\mathcal{B}(\Omega), \mathbf{v} \rangle = \int_{\partial \Omega} \text{Tr}(i_{\mathbf{v}}(* \mathbf{d} \omega \wedge \mathbf{d} \boldsymbol{\eta})) + \int_{\Omega} * \mathbf{d} \delta \omega \wedge \mathbf{d} \boldsymbol{\eta} + \int_{\Omega} * \mathbf{d} \omega \wedge \mathbf{d} \delta \boldsymbol{\eta} , \quad (4.9)$$

*where  $*$  is a Hodge star operator and  $\delta \omega, \delta \boldsymbol{\eta} \in \mathbf{H}(\mathbf{d}, \Omega_R, \wedge^l(\mathbb{R}^d))$  are the shape derivatives as introduced in Definition 1.2.*

*Proof.* Apply Lemma 4.1 to the shape-dependent  $d$ -form  $D \mapsto * \mathbf{d} \omega(D) \wedge \mathbf{d} \boldsymbol{\eta}(D)$ .  $\square$

We are now in a position to derive shape derivatives of solutions to abstract scattering problems case-by-case.

**4.3. Impedance and Neumann boundary conditions.** Now we examine the shape derivative of the solution  $\omega = \omega(\Omega)$  of the variational problem (3.15). To begin with we point out that the truncation boundary  $\Gamma_R$  is fixed and that test forms  $\boldsymbol{\eta}$  never depend on  $\Omega$ . Our policy is to apply Lemmas 4.1 and 4.3 to (3.15). Certain complications arise in the case of the boundary term

$$B(\Omega) := \int_{\Gamma} *_{\lambda}^{\Gamma}(\text{Tr} \omega(\Omega)) \wedge \text{Tr} \boldsymbol{\eta} , \quad \Gamma := \partial \Omega , \quad (4.10)$$

because there is a hidden dependence on  $\Omega$  in the surface Hodge operator  $*_{\lambda}^{\Gamma}$ . This becomes apparent, when using Assumption 1 and (3.3) to recast (4.10) as

$$B(\Omega) = \lambda \int_{\Gamma} \text{Tr}(i_{\mathbf{n}}(*\omega(\Omega)) \wedge \boldsymbol{\eta}) . \quad (4.11)$$

Clearly the outward unit normal vector  $\mathbf{n}$  will be affected by a perturbation of  $\Omega$ :  $\mathbf{n} = \mathbf{n}(\Omega)$  so that dependence on  $\Omega$  enters  $B(\Omega)$  in three ways through  $\Gamma = \Gamma(\Omega)$ ,  $\mathbf{n} = \mathbf{n}(\Omega)$ , and  $\omega = \omega(\Omega)$ . Since  $B(\Omega)$  is linear both in  $\mathbf{n}$  and  $\omega$ , the chain rule combined with (4.7) yields

$$\langle dB(\Omega), \mathbf{v} \rangle = \lambda \int_{\Gamma} \text{Tr} (i_{\mathbf{v}} \mathbf{d} (i_{\mathbf{n}}(*\omega) \wedge \eta)) + \lambda \int_{\Gamma} \text{Tr} (i_{\delta \mathbf{n}}(*\omega) \wedge \eta) + \int_{\Gamma} *_{\lambda}^{\Gamma} (\text{Tr} \delta \omega) \wedge \eta. \quad (4.12)$$

Here  $\delta \mathbf{n}$  is the shape derivative of the exterior unit normal to  $\Gamma$  [7, IX (4.38)]

$$\delta \mathbf{n}|_{\Gamma} = \{(\mathbf{n}^{\top} D\mathbf{v} \mathbf{n}) \mathbf{n} - D\mathbf{v}^{\top} \mathbf{n} - D\mathbf{n} \mathbf{v}\}|_{\Gamma} = - (D\mathbf{v}^{\top} \mathbf{n})_{\mathbf{t}} - \{D\mathbf{n} \mathbf{v}\}|_{\Gamma},$$

where  $(\cdot)_{\mathbf{t}}$  picks the tangential components on  $\Gamma$ . The Jacobian of  $\mathbf{n}$  is the Weingarten map  $D\mathbf{n}$ , which sends any vector  $\mathbf{v}$  to a vector tangential to  $\Gamma$  [7, IX.5.6]. Hence, the entire expression is tangential and can be rewritten as a tangential gradient

$$\delta \mathbf{n}|_{\Gamma} = - \mathbf{grad}_{\Gamma}(\mathbf{v} \cdot \mathbf{n}). \quad (4.13)$$

The third term of (4.12) is present in the bilinear form  $a_I$ . Thus, we arrive at the variational characterization of the shape derivative  $\delta \omega$  of the solution  $\omega$  of the variational problem (3.15):

**THEOREM 4.4.** *The shape derivative  $\delta \omega := \langle \delta \omega, \mathbf{v} \rangle$  of the solution  $\omega = \omega(\Omega) \in \mathbf{H}^1(\mathbf{d}, \Omega^e, \wedge^l(\mathbb{R}^d))$  of the impedance/Neumann boundary value problem (3.1) with (3.2c)/(3.2b) is the unique solution of the variational problem: seek  $\delta \omega \in \mathbf{H}(\mathbf{d}, \Omega^e, \wedge^l(\mathbb{R}^d))$  such that*

$$a_I(\delta \omega, \eta) = - \int_{\Gamma} \text{Tr} i_{\mathbf{v}} (*_{\alpha} \mathbf{d} \omega \wedge \mathbf{d} \eta - *_{\kappa} \omega \wedge \eta) - \text{i} \lambda \int_{\Gamma} \text{Tr} i_{\mathbf{v}} \mathbf{d} (i_{\mathbf{n}}(*\omega) \wedge \eta) - \text{i} \lambda \int_{\Gamma} \text{Tr} (i_{\delta \mathbf{n}}(*\omega) \wedge \eta). \quad (4.14)$$

for all  $\eta \in \mathcal{DF}^{l, \infty}(\Omega_R)$ .

Note that the trial space in (4.14) is appropriate due to the regularity of the shape derivative guaranteed by Corollary 3.1. In addition, the regularity  $\omega \in \mathbf{H}^1(\mathbf{d}, \Omega^e, \wedge^l(\mathbb{R}^d))$  provided by Assumption 2 ensures that the right hand side of (4.14) is well defined.

The first two terms of the right hand side of (4.14) allow substantial simplifications. Key steps involve the product rules [9],

$$i_{\mathbf{v}}(\omega \wedge \eta) = i_{\mathbf{v}} \omega \wedge \eta + (-1)^{\deg(\omega)} \omega \wedge i_{\mathbf{v}} \eta, \quad (4.15)$$

$$\mathbf{d}(\omega \wedge \eta) = \mathbf{d} \omega \wedge \eta + (-1)^{\deg(\omega)} \omega \wedge \mathbf{d} \eta, \quad (4.16)$$

where  $\deg(\omega)$  is the degree of the form  $\omega$ . Thus we have for  $l$ -forms  $\omega$  and  $\eta$

$$\mathbf{d}(i_{\mathbf{n}}(*\omega) \wedge \eta) = \mathbf{d}(i_{\mathbf{n}}(*\omega)) \wedge \eta + (-1)^{d-l-1} i_{\mathbf{n}}(*\omega) \wedge (\mathbf{d} \eta). \quad (4.17)$$

We apply this to the first two terms of the right hand side of (4.14), use (4.15) repeatedly, and cancel terms that vanish due to the impedance boundary condition (3.2c), which yields

$$\begin{aligned} & - \int_{\Gamma} i_{\mathbf{v}} (*_{\alpha} \mathbf{d} \omega \wedge \mathbf{d} \eta - *_{\kappa} \omega \wedge \eta + \text{i} \lambda \mathbf{d} (i_{\mathbf{n}}(*\omega) \wedge \eta)) \\ \stackrel{(4.17)}{=} & - \int_{\Gamma} i_{\mathbf{v}} ((*_{\alpha} \mathbf{d} \omega \wedge \mathbf{d} \eta + \text{i} \lambda (-1)^{d-l-1} (i_{\mathbf{n}}(*\omega)) \wedge (\mathbf{d} \eta)) - *_{\kappa} \omega \wedge \eta + \text{i} \lambda \mathbf{d}(i_{\mathbf{n}}(*\omega)) \wedge \eta) \end{aligned}$$

$$\begin{aligned}
&\stackrel{(4.15)}{=} - \int_{\Gamma} (\mathbf{v} \cdot \mathbf{n}) \operatorname{Tr} \left\{ i_{\mathbf{n}} (*_{\alpha} \mathbf{d} \boldsymbol{\omega} + \underbrace{i\lambda(-1)^{d-l-1} i_{\mathbf{n}}(*\boldsymbol{\omega})}_{\text{drop, since } i_{\mathbf{n}} i_{\mathbf{n}}=0}) \right\} \wedge (\mathbf{d} \boldsymbol{\eta}) - (\mathbf{v} \cdot \mathbf{n}) \operatorname{Tr} (i_{\mathbf{n}} (*_{\kappa} \boldsymbol{\omega} \wedge \boldsymbol{\eta})) \\
&\quad - (-1)^{d-l-1} \int_{\Gamma} (\mathbf{v} \cdot \mathbf{n}) \underbrace{(\operatorname{Tr}(*_{\alpha} \mathbf{d} \boldsymbol{\omega}) + i\lambda(-1)^{d-l-1} *^{\Gamma} \operatorname{Tr} \boldsymbol{\omega})}_{=0 \text{ by IBC.}} \wedge \operatorname{Tr} (i_{\mathbf{n}}(\mathbf{d} \boldsymbol{\eta})) \\
&\quad - i\lambda(-1)^{d-l-1} \int_{\Gamma} (\mathbf{v} \cdot \mathbf{n}) \operatorname{Tr} (i_{\mathbf{n}}(\mathbf{d}(i_{\mathbf{n}}(*\boldsymbol{\omega}))) \wedge \boldsymbol{\eta})) \\
&\stackrel{(4.15)}{=} - \int_{\Gamma} (\mathbf{v} \cdot \mathbf{n}) \left\{ \operatorname{Tr} (i_{\mathbf{n}} (*_{\alpha} \mathbf{d} \boldsymbol{\omega}) \wedge (\mathbf{d} \boldsymbol{\eta})) - \operatorname{Tr} (i_{\mathbf{n}}(*_{\kappa} \boldsymbol{\omega}) \wedge \boldsymbol{\eta} + (-1)^{d-l} *_{\kappa} \boldsymbol{\omega} \wedge (i_{\mathbf{n}} \boldsymbol{\eta})) + \right. \\
&\quad \left. i\lambda \operatorname{Tr} (i_{\mathbf{n}}(\mathbf{d}(i_{\mathbf{n}}(*\boldsymbol{\omega}))) \wedge \boldsymbol{\eta}) - (-1)^{d-l-1} \mathbf{d}(i_{\mathbf{n}}(*\boldsymbol{\omega})) \wedge (i_{\mathbf{n}} \boldsymbol{\eta})) \right\} \\
&\stackrel{(3.5)}{=} - \int_{\Gamma} (\mathbf{v} \cdot \mathbf{n}) \left\{ \operatorname{Tr} (i_{\mathbf{n}} (*_{\alpha} \mathbf{d} \boldsymbol{\omega}) \wedge (\mathbf{d} \boldsymbol{\eta})) - \operatorname{Tr} (i_{\mathbf{n}}(*_{\kappa} \boldsymbol{\omega}) \wedge (\operatorname{Tr} \boldsymbol{\eta})) + \right. \\
&\quad \left. i\lambda \operatorname{Tr} (i_{\mathbf{n}}(\mathbf{d}(i_{\mathbf{n}}(*\boldsymbol{\omega}))) \wedge \boldsymbol{\eta}) \right\} \\
&\stackrel{(*)}{=} \int_{\Gamma} (-1)^l \mathbf{d}_{\Gamma} \{ (\mathbf{v} \cdot \mathbf{n}) \operatorname{Tr} i_{\mathbf{n}} (*_{\alpha} \mathbf{d} \boldsymbol{\omega}) \} \wedge \boldsymbol{\eta} + \\
&\quad \int_{\Gamma} (\mathbf{v} \cdot \mathbf{n}) \left\{ \operatorname{Tr} (i_{\mathbf{n}}(*_{\kappa} \boldsymbol{\omega}) \wedge \boldsymbol{\eta}) - i\lambda \operatorname{Tr} (i_{\mathbf{n}}(\mathbf{d}(i_{\mathbf{n}}(*\boldsymbol{\omega}))) \wedge \boldsymbol{\eta}) \right\} .
\end{aligned}$$

In Step (\*) we performed integration by parts on the closed surface  $\Gamma$ . Summing up, we have found a representation of the right hand side functional of (4.14):

$$\begin{aligned}
&- \int_{\Gamma} \operatorname{Tr} i_{\mathbf{v}} (*_{\alpha} \mathbf{d} \boldsymbol{\omega} \wedge \mathbf{d} \boldsymbol{\eta} - *_{\kappa} \boldsymbol{\omega} \wedge \boldsymbol{\eta}) - \\
&\quad i\lambda \int_{\Gamma} \operatorname{Tr} i_{\mathbf{v}} \mathbf{d} (i_{\mathbf{n}}(*\boldsymbol{\omega}) \wedge \boldsymbol{\eta}) - i\lambda \int_{\Gamma} \operatorname{Tr} (i_{\delta \mathbf{n}}(*\boldsymbol{\omega}) \wedge \boldsymbol{\eta}) = \int_{\Gamma} T(\boldsymbol{\omega}) \wedge \operatorname{Tr}(\boldsymbol{\eta}) ,
\end{aligned}$$

with

$$\begin{aligned}
T(\boldsymbol{\omega}) &:= (-1)^l \mathbf{d}_{\Gamma} \{ (\mathbf{v} \cdot \mathbf{n}) \operatorname{Tr} i_{\mathbf{n}} (*_{\alpha} \mathbf{d} \boldsymbol{\omega}) \} + \\
&\quad (\mathbf{v} \cdot \mathbf{n}) \left\{ \operatorname{Tr} (i_{\mathbf{n}}(*_{\kappa} \boldsymbol{\omega})) - i\lambda \operatorname{Tr} (i_{\mathbf{n}}(\mathbf{d}(i_{\mathbf{n}}(*\boldsymbol{\omega})))) \right\} - i\lambda \operatorname{Tr} (i_{\delta \mathbf{n}}(*\boldsymbol{\omega})) .
\end{aligned} \tag{4.18}$$

We recall an immediate consequence of the integration by parts formula:

LEMMA 4.5. *If  $\zeta \in \mathbf{H}(\mathbf{d}, \Omega, \wedge^l(\mathbb{R}^d))$  then  $\boldsymbol{\eta} \mapsto \int_{\Gamma} \operatorname{Tr} \zeta \wedge \operatorname{Tr} \boldsymbol{\eta}$  is continuous on  $\mathbf{H}(\mathbf{d}, \Omega, \wedge^l(\mathbb{R}^d))$ .*

Combined with the prior manipulations, this reveals that the right-hand-side of (4.14), viewed as a function of  $\boldsymbol{\eta}$ , provides a *continuous* linear form on  $\mathbf{H}(\mathbf{d}, \Omega^e, \wedge^l(\mathbb{R}^d))$ , if  $\boldsymbol{\omega} \in \mathbf{H}^1(\mathbf{d}, \Omega^e, \wedge^l(\mathbb{R}^d))$ . Hence, thanks to Assumption 2,  $V := \{ \boldsymbol{\omega} \in \mathbf{H}(\mathbf{d}, \Omega^e, \wedge^l(\mathbb{R}^d)), \operatorname{Tr}(\boldsymbol{\omega}) \in \mathbf{L}^2(\Gamma, \wedge^l(\Gamma)) \}$  remains a valid trial space for (4.14). In the case  $\lambda = 0$  we may even use  $\boldsymbol{\eta} \in \mathbf{H}(\mathbf{d}, \Omega^e, \wedge^l(\mathbb{R}^d))$ .

The simplified form of the right hand side of (4.14) also gives the strong form of the impedance/Neumann boundary value problem satisfied by the shape gradient. It boils down to (3.1) (replacing  $\boldsymbol{\omega}$  with  $\delta \boldsymbol{\omega}$ ) with  $g = 0$ , but non-homogeneous impedance/Neumann conditions  $BC(\delta \boldsymbol{\omega}) = T(\boldsymbol{\omega})$ , where  $T(\boldsymbol{\omega})$  is defined in (4.18).

REMARK 1. *Beside Assumption 1 let us assume that everywhere  $\alpha$  and  $\kappa$  are just scalar multiples of the Euclidean metric. Then (3.3) allows the reformulation*

$$\begin{aligned}
T(\boldsymbol{\omega}) &= (-1)^l \mathbf{d}_{\Gamma} \{ (\mathbf{v} \cdot \mathbf{n}) \alpha *^{\Gamma} \mathbf{d}_{\Gamma} \operatorname{Tr} \boldsymbol{\omega} \} + \\
&\quad (\mathbf{v} \cdot \mathbf{n}) \left\{ \kappa *^{\Gamma} \operatorname{Tr} \boldsymbol{\omega} - i\lambda \operatorname{Tr} (i_{\mathbf{n}}(\mathbf{d}(i_{\mathbf{n}}(*\boldsymbol{\omega})))) \right\} - i\lambda \operatorname{Tr} (i_{\delta \mathbf{n}}(*\boldsymbol{\omega})) ,
\end{aligned} \tag{4.19}$$

where  $*^\Gamma$  is the surface Hodge induced by the Euclidean volume Hodge  $*$  and, abusing notation,  $\alpha$  and  $\kappa$  now designate coefficient functions.

**4.4. Dirichlet boundary conditions.** The variational saddle point problem (3.19) is amenable to a direct application of Lemma 4.3 to all its bilinear forms, which yields

$$\begin{aligned} \mathfrak{a}_D \left( \begin{pmatrix} \delta \boldsymbol{\rho} \\ \delta \boldsymbol{\omega} \end{pmatrix}, \begin{pmatrix} \boldsymbol{\tau} \\ \boldsymbol{\nu} \end{pmatrix} \right) &= - \int_{\Gamma} \text{Tr} i_{\mathbf{v}} (*_{\alpha^{-1}} \boldsymbol{\rho} \wedge \boldsymbol{\tau} + (-1)^{(l+1)d+1} \boldsymbol{\omega} \wedge \mathbf{d} \boldsymbol{\tau}) - \\ &\quad \int_{\Gamma} \text{Tr} i_{\mathbf{v}} \underbrace{((-1)^{d-l} \mathbf{d} \boldsymbol{\rho} \wedge \boldsymbol{\nu} - *_{\kappa} \boldsymbol{\omega} \wedge \boldsymbol{\nu})}_{=0, \text{ due to (3.1a)}}. \end{aligned} \quad (4.20)$$

for any  $\boldsymbol{\tau} \in \mathcal{DF}^{d-l-1, \infty}(\Omega_R)$  and  $\boldsymbol{\nu} \in \mathcal{DF}^{d-l, \infty}(\Omega_R)$ . Then we can use (3.17), (4.15) and the Dirichlet boundary condition  $\text{Tr} \boldsymbol{\omega} = 0$  to simplify the equations. Again, keep in mind that the test forms do not depend on  $\Omega$  nor does  $\Gamma_R$ . Thus we arrive at the following result, extending what we got in [20, Section 6]:

**THEOREM 4.6.** *The shape derivative  $\delta \boldsymbol{\omega}$  of the solution  $\boldsymbol{\omega}$  of the Dirichlet boundary value problem (3.1) and (3.2a) is given as the unique solution of the variational problem: seek  $\delta \boldsymbol{\omega} \in \mathbf{L}^2(\Omega^e, \wedge^l(\mathbb{R}^d))$  and  $\delta \boldsymbol{\rho} \in \mathbf{H}(\mathbf{d}, \Omega^e, \wedge^{d-l-1}(\mathbb{R}^d))$  such that*

$$\mathfrak{a}_D \left( \begin{pmatrix} \delta \boldsymbol{\rho} \\ \delta \boldsymbol{\omega} \end{pmatrix}, \begin{pmatrix} \boldsymbol{\tau} \\ \boldsymbol{\nu} \end{pmatrix} \right) = -(-1)^{(l+1)(d-1)} \int_{\Gamma} \text{Tr}(i_{\mathbf{v}} \mathbf{d} \boldsymbol{\omega}) \wedge \boldsymbol{\tau} + (-1)^l \text{Tr}(i_{\mathbf{v}} \boldsymbol{\omega}) \wedge \mathbf{d} \boldsymbol{\tau}. \quad (4.21)$$

for all  $\boldsymbol{\tau} \in \mathcal{DF}^{d-l-1, \infty}(\overline{\Omega}_R)$  and  $\boldsymbol{\nu} \in \mathcal{DF}^{d-l, \infty}(\overline{\Omega}_R)$ .

In light of Corollary 3.1 the function spaces chosen for (4.21) capture the shape derivative. Since  $\boldsymbol{\omega} \in \mathbf{H}^1(\mathbf{d}, \Omega^e, \wedge^l(\mathbb{R}^d))$  thanks to Assumption 2, the expression on the right hand side of (4.21) is a bounded linear form on  $\mathbf{H}(\mathbf{d}, \Omega_R, \wedge^{d-l-1}(\mathbb{R}^d))$  according to Lemma 4.5.

In order to identify the Dirichlet boundary conditions hidden in (4.21), we perform integration by parts on  $\Gamma$  and get

$$\begin{aligned} \int_{\Gamma} \text{Tr}(i_{\mathbf{v}} \mathbf{d} \boldsymbol{\omega} \wedge \boldsymbol{\tau} + (-1)^l i_{\mathbf{v}} \boldsymbol{\omega} \wedge \mathbf{d} \boldsymbol{\tau}) &= \int_{\Gamma} (\text{Tr}(i_{\mathbf{v}} \mathbf{d} \boldsymbol{\omega}) - \mathbf{d}_{\Gamma} \text{Tr}(i_{\mathbf{v}} \boldsymbol{\omega})) \wedge \boldsymbol{\tau} \\ &= \int_{\Gamma} \underbrace{((\mathbf{v} \cdot \mathbf{n}) \text{Tr}(i_{\mathbf{n}} \mathbf{d} \boldsymbol{\omega}) - \mathbf{d}_{\Gamma} \{(\mathbf{v} \cdot \mathbf{n}) \text{Tr}(i_{\mathbf{n}} \boldsymbol{\omega})\})}_{=: G(\boldsymbol{\omega})} \wedge \boldsymbol{\tau}. \end{aligned} \quad (4.22)$$

Here, in principle,  $\mathbf{n}$  can be any transversal  $C^1$ -vector field on  $\Gamma$ . Hence, the strong form of (4.21) comprises the PDE (3.1a) replacing  $\boldsymbol{\omega}$  with  $\delta \boldsymbol{\omega}$ , the homogeneous absorbing boundary condition  $ABC(\delta \boldsymbol{\omega}) = 0$ , and an inhomogeneous Dirichlet boundary condition  $\text{Tr}(\delta \boldsymbol{\omega}) = G(\boldsymbol{\omega})$  on  $\Gamma$ .

**4.5. Transmission case.** Like the impedance case, applying Lemmas 4.1 and 4.3 to the bilinear forms of (3.21) yields a variational characterization of the shape derivative  $\delta \boldsymbol{\omega}$  for the solution  $\boldsymbol{\omega} = \boldsymbol{\omega}(\Omega)$  as defined in (3.23). The opposite induced orientations of  $\Gamma$  when viewed from  $\Omega$  and  $\Omega^e$  engender jumps, see (3.8) for their definition.

**THEOREM 4.7.** *The shape derivative  $\langle \delta \boldsymbol{\omega}, \mathbf{v} \rangle$  of the solution  $\boldsymbol{\omega}$  of the transmission problem (3.6), (3.7) can be obtained by restricting the solutions of the following variational problem to the respective domains  $\Omega$  and  $\Omega^e$ : seek  $\delta \boldsymbol{\omega}^e \in \mathbf{H}(\mathbf{d}, \Omega_R, \wedge^l(\mathbb{R}^d))$ ,  $\delta \boldsymbol{\omega}^i \in \mathbf{H}(\mathbf{d}, \Omega_R, \wedge^l(\mathbb{R}^d))$  such that for all smooth test forms  $\boldsymbol{\eta} \in \mathcal{DF}^{l, \infty}(\overline{\Omega}_R)$ ,  $\boldsymbol{\mu} \in \mathcal{DF}^{d-l-1, \infty}(\overline{\Omega}_R)$*

$$a_T \left( \begin{pmatrix} \delta\omega^e \\ \delta\omega^i \end{pmatrix}, \begin{pmatrix} \eta \\ \mu \end{pmatrix} \right) = - \int_{\Gamma} \text{Tr } i_{\mathbf{v}} \left( [(*_{\alpha} \mathbf{d}\omega)]_{\Gamma} \wedge \mathbf{d}\eta - [*_{\kappa}\omega]_{\Gamma} \wedge \eta \right) + \text{Tr} (i_{\mathbf{v}} \mathbf{d}[\omega]_{\Gamma}) \wedge \mu + \mathbf{d}_{\Gamma} \text{Tr} (i_{\mathbf{v}} [\omega]_{\Gamma}) \wedge \mu. \quad (4.23)$$

In light of Corollary 3.1 the trial space of (4.23) contains the shape derivative  $\langle \delta\omega, \mathbf{v} \rangle$ . Further, Assumption 2 ensures that the right hand side of (4.23) is well defined.

In order to state the strong form of the transmission problem described by (4.23) the following results tells us how to extract transmission conditions.

LEMMA 4.8. *If  $\omega^e \in \mathbf{H}(\mathbf{d}, \Omega_R, \wedge^l(\mathbb{R}^d))$  and  $\omega^i \in \mathbf{H}(\mathbf{d}, \Omega_R, \wedge^l(\mathbb{R}^d))$  satisfy*

$$a_T \left( \begin{pmatrix} \omega^e \\ \omega^i \end{pmatrix}, \begin{pmatrix} \eta \\ \mu \end{pmatrix} \right) = \int_{\Gamma} \gamma \wedge \eta + \zeta \wedge \mu \quad (4.24)$$

for all  $\eta \in \mathcal{DF}^{l,\infty}(\overline{\Omega}_R)$ ,  $\mu \in \mathcal{DF}^{d-l-1,\infty}(\overline{\Omega}_R)$ , and some  $d-l-1$ -form  $\gamma$  and an  $l$ -form  $\zeta$ , then  $\omega^i$  and  $\omega^e$  satisfy (3.6a) and (3.6b), respectively, and, defining  $\omega$  as in (3.23),

$$[\text{Tr } \omega]_{\Gamma} = \zeta \quad \text{and} \quad [\text{Tr } *_{\alpha} \mathbf{d}\omega]_{\Gamma} = \gamma. \quad (4.25)$$

Thus, we have to match the right hand sides of (4.23) and (4.24). Focusing on the  $\mu$ -dependent terms, it is immediate that

$$\begin{aligned} [\text{Tr } \delta\omega]_{\Gamma} &= \text{Tr} (i_{\mathbf{v}} \mathbf{d}[\omega]_{\Gamma}) + \mathbf{d}_{\Gamma} \text{Tr} (i_{\mathbf{v}} [\omega]_{\Gamma}) \\ &= (\mathbf{v} \cdot \mathbf{n}) \text{Tr} (i_{\mathbf{n}} \mathbf{d}[\omega]_{\Gamma}) + \mathbf{d}_{\Gamma} \{ (\mathbf{v} \cdot \mathbf{n}) i_{\mathbf{n}} [\omega]_{\Gamma} \}, \end{aligned} \quad (4.26)$$

with some transversal  $C^1$ -vector field  $\mathbf{n}$  on  $\Gamma$ . Next, we manipulate the first term on the right hand side of (4.23):

$$\begin{aligned} \text{Tr } i_{\mathbf{v}} \left( [(*_{\alpha} \mathbf{d}\omega)]_{\Gamma} \wedge \mathbf{d}\eta - [*_{\kappa}\omega]_{\Gamma} \wedge \eta \right) &= \\ \text{Tr} \left\{ i_{\mathbf{v}} [*_{\alpha} \mathbf{d}\omega]_{\Gamma} \wedge \mathbf{d}\eta + (-1)^{d-l-1} [*_{\alpha} \mathbf{d}\omega]_{\Gamma} \wedge i_{\mathbf{v}} \mathbf{d}\eta - \right. & (4.27) \\ \left. i_{\mathbf{v}} [*_{\kappa}\omega]_{\Gamma} \wedge \eta - (-1)^{d-l} [*_{\kappa}\omega]_{\Gamma} \wedge i_{\mathbf{v}} \eta \right\}. \end{aligned}$$

By virtue of the transmission conditions (3.7)

$$\text{Tr} [*_{\alpha} \mathbf{d}\omega]_{\Gamma} = 0 \quad \Rightarrow \quad \text{Tr} [*_{\kappa}\omega]_{\Gamma} = (-1)^{d-l} \mathbf{d}_{\Gamma} \text{Tr} [*_{\alpha} \mathbf{d}\omega]_{\Gamma} = 0.$$

Therefore, two terms can be dropped from (4.27) and after integration by parts we eventually get

$$\begin{aligned} \text{Tr } i_{\mathbf{v}} \left( [(*_{\alpha} \mathbf{d}\omega)]_{\Gamma} \wedge \mathbf{d}\eta - [*_{\kappa}\omega]_{\Gamma} \wedge \eta \right) &= \\ \{ (-1)^{d-l} \mathbf{d}_{\Gamma} \text{Tr} (i_{\mathbf{v}} [*_{\alpha} \mathbf{d}\omega]_{\Gamma}) - \text{Tr} (i_{\mathbf{v}} [*_{\kappa}\omega]_{\Gamma}) \} \wedge \eta. \end{aligned} \quad (4.28)$$

Appealing to Lemma 4.8 we have found

$$\begin{aligned} \text{Tr} [*_{\alpha} \mathbf{d}\delta\omega]_{\Gamma} &= (-1)^{d-l} \mathbf{d}_{\Gamma} [\text{Tr } i_{\mathbf{v}} *_{\alpha} \mathbf{d}\omega]_{\Gamma} - [\text{Tr } i_{\mathbf{v}} *_{\kappa} \omega]_{\Gamma} \\ &= (-1)^{d-l} \mathbf{d}_{\Gamma} \{ (\mathbf{v} \cdot \mathbf{n}) [\text{Tr } i_{\mathbf{n}} *_{\alpha} \mathbf{d}\omega]_{\Gamma} \} - (\mathbf{v} \cdot \mathbf{n}) [\text{Tr } i_{\mathbf{n}} *_{\kappa} \omega]_{\Gamma}. \end{aligned} \quad (4.29)$$

Moreover, invoking Lemma 4.5 again, under Assumption 2 the right hand side of (4.23) turns out to be continuous on  $\mathbf{H}(\mathbf{d}, \Omega_R, \wedge^l(\mathbb{R}^d)) \times \mathbf{H}(\mathbf{d}, \Omega_R, \wedge^{d-l-1}(\mathbb{R}^d))$  so that these two test spaces can be used in (4.23).

In sum, the strong form of (4.23) comprises the PDE (3.6a)-(3.6b) replacing  $\omega^m$  with  $\delta\omega^m$ ,  $m = i$  or  $e$ , respectively, the homogeneous absorbing boundary condition  $ABC(\delta\omega) = 0$ , and two inhomogeneous transmission conditions given by (4.26) and (4.29).

**5. Shape derivatives in vector proxies in 3D.** In this section, we will translate the results from Section 4 to classical vector calculus that has prevailed in shape calculus so far. We emphasize that vector calculus provides an isomorphic model for exterior calculus after having fixed coordinates.

**5.1. Vector proxies.** The variational formulation for time-harmonic acoustic and electromagnetic scattering problems can be expressed in the language of classical vector calculus after switching to the (Euclidean) vector proxy incarnation of differential forms, see, e.g., [18–20]. Refer to Tables 5.1 and 5.2 and [19] for how to relate differential forms and their vector proxy representatives in 3D domains and on 2D oriented manifolds embedded in  $\mathbb{R}^3$ . In 3D exterior derivatives and contractions boil down to familiar operations for Euclidean vector proxies, see Table 5.3.

$l$	Differential forms, degree $l$	Related function $u$ / vector field $\mathbf{u}$
0	$\mathbf{x} \mapsto \omega(\mathbf{x})$	$u(\mathbf{x}) := \omega(\mathbf{x})$
1	$\mathbf{x} \mapsto \{\mathbf{v} \mapsto \omega(\mathbf{x})(\mathbf{v})\}$	$\langle \mathbf{u}(\mathbf{x}), \mathbf{v} \rangle := \omega(\mathbf{x})(\mathbf{v})$
2	$\mathbf{x} \mapsto \{\mathbf{v}_1, \mathbf{v}_2 \mapsto \omega(\mathbf{x})(\mathbf{v}_1, \mathbf{v}_2)\}$	$\langle \mathbf{u}(\mathbf{x}), \mathbf{v}_1 \times \mathbf{v}_2 \rangle := \omega(\mathbf{x})(\mathbf{v}_1, \mathbf{v}_2)$
3	$\mathbf{x} \mapsto \{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3 \mapsto \omega(\mathbf{x})(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)\}$	$u(\mathbf{x}) \det(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3) := \omega(\mathbf{x})(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)$

Table 5.1: Relationship between differential forms and Euclidean vector proxies in a 3D domain  $\Omega$ .  $\mathbf{v}, \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3 \in \mathbb{R}^3$ .

	Differential forms, degree $l$	Related function $u$ / vector field $\mathbf{u}$
$l = 0$	$\mathbf{x} \mapsto \omega(\mathbf{x})$	$u(\mathbf{x}) := \omega(\mathbf{x})$
$l = 1$	$\mathbf{x} \mapsto \{\mathbf{v} \mapsto \omega(\mathbf{x})(\mathbf{v})\}$	$\langle \mathbf{u}(\mathbf{x}), \mathbf{v} \rangle := \omega(\mathbf{x})(\mathbf{v})$
$l = 2$	$\mathbf{x} \mapsto \{\mathbf{v}_1, \mathbf{v}_2 \mapsto \omega(\mathbf{x})(\mathbf{v}_1, \mathbf{v}_2)\}$	$u(\mathbf{x}) \det(\mathbf{v}_1, \mathbf{v}_2, \mathbf{n}) := \omega(\mathbf{x})(\mathbf{v}_1, \mathbf{v}_2)$

Table 5.2: Relationship between differential forms and vector proxies in a 2D oriented manifold  $\Gamma$  of codimension one embedded in  $\mathbb{R}^3$ .  $\mathbf{v}, \mathbf{v}_1$ , and  $\mathbf{v}_2$  are to be taken from the tangent space at  $\Gamma$  in  $\mathbf{x}$  and  $\mathbf{n}$  is the unit outward normal to  $\Gamma$ .

	3D				2D (on surface $\Gamma$ )		
$l$	0	1	2	3	0	1	2
$\mathbf{d}\omega$	$\mathbf{grad} u$	$\mathbf{curl} \mathbf{u}$	$\mathbf{div} \mathbf{u}$	0	$\mathbf{grad}_\Gamma$	$\mathbf{curl}_\Gamma$	0
$i_{\mathbf{v}}\omega$	0	$\mathbf{u} \cdot \mathbf{v}$	$\mathbf{u} \times \mathbf{v}$	$u\mathbf{v}$	0	$\mathbf{u} \cdot \mathbf{v}$	$u(\mathbf{v} \times \mathbf{n})$

Table 5.3: Operators of exterior calculus in their Euclidean vector proxy incarnations. Function  $u$  and vector field  $\mathbf{u}$  stand for the vector proxies of the  $l$ -form  $\omega$ .

In this section we assume that all Hodge operators are induced by metrics that are scalar multiples of the Euclidean metric. Thus all Hodge operators become scalar multiples of a single Euclidean Hodge operator  $*$  and, for instance,  $*_\alpha = \alpha \cdot *$ , where  $\alpha = \alpha(\mathbf{x})$  is a positive smooth function on  $\Omega_R$ . Moreover,  $\lambda$  will be set equal to a positive constant. Then,

Table 5.4: Boundary value problems (3.1) and transmission problems (3.6) for acoustic scattering, that is,  $l = 0$ .

PDE	Obstacle scattering	$-\mathbf{div}(\alpha \mathbf{grad} u) - \kappa u = 0$ in $\Omega^e$
	Medium scattering	$\begin{cases} -\mathbf{div}(\alpha_i \mathbf{grad} u) - \kappa_i u = 0 & \text{in } \Omega \\ -\mathbf{div}(\alpha_e \mathbf{grad} u) - \kappa_e u = 0 & \text{in } \Omega^e \end{cases}$
BC /IC on $\Gamma$	Sound-soft	$u = 0$
	Sound-hard	$\alpha \frac{\partial u}{\partial \mathbf{n}} = 0$
	Impedance	$\alpha \frac{\partial u}{\partial \mathbf{n}} + i\lambda \delta u = 0$
	Transmission	$\begin{cases} [u] = 0 \\ [\alpha \frac{\partial u}{\partial \mathbf{n}}] = 0 \end{cases}$

Table 5.5: Boundary value problems (3.1) and transmission problems (3.6) for electromagnetic scattering, that is,  $l = 1$ .

PDE	Obstacle scattering	$\mathbf{curl}(\alpha \mathbf{curl} \mathbf{E}) - \kappa \mathbf{E} = 0$ in $\Omega^e$
	Medium scattering	$\begin{cases} \mathbf{curl}(\alpha_i \mathbf{curl} \mathbf{E}) - \kappa_i \mathbf{E} = 0 & \text{in } \Omega \\ \mathbf{curl}(\alpha_e \mathbf{curl} \mathbf{E}) - \kappa_e \mathbf{E} = 0 & \text{in } \Omega^e \end{cases}$
BC /IC on $\Gamma$	PEC	$\mathbf{n} \times \mathbf{E} = 0$
	PMC	$\alpha \mathbf{n} \times (\mathbf{curl} \mathbf{E}) = 0$
	Impedance	$\alpha \mathbf{n} \times (\mathbf{curl} \mathbf{E}) - i\lambda \mathbf{E}_T = 0$
	Transmission	$\begin{cases} [\mathbf{n} \times \mathbf{E}] = 0 \\ [\alpha \mathbf{n} \times (\mathbf{curl} \mathbf{E})] = 0 \end{cases}$

for 3D vector proxies, the application of a Hodge operator just amounts to pointwise scalar multiplication with its associated function.

Using this fact and the translation tables, it is easy to state the 3D vector proxy versions of all relevant boundary value problems (3.1) and transmission problems (3.6). They are summarized in Tables 5.4 and 5.5. As usual, we gloss over radiation conditions.

For later use, we recall surface differential operators, *cf.* [7, § 9.5], some of which incarnate the exterior derivative on surfaces, see Table 5.3. Let  $\tilde{u}$  (resp.  $\tilde{\mathbf{v}}$ ) be the classical extension of some scalar function  $u$  (resp. vector field  $\mathbf{v}$ ) on the surface  $\Gamma$  to a neighborhood of  $\Gamma$  by means of the signed smooth distance function [7, 31, 36]. Then we define the

$$\begin{aligned} \text{surface gradient : } \mathbf{grad}_\Gamma u &:= \mathbf{grad} \tilde{u}|_\Gamma - (\mathbf{grad} \tilde{u} \cdot \mathbf{n}) \mathbf{n}|_\Gamma, \\ \text{surface curl : } \mathbf{curl}_\Gamma u &:= \mathbf{grad} \tilde{u} \times \mathbf{n}, \end{aligned}$$

$$\begin{aligned} \text{scalar curl : } & \text{curl}_\Gamma \mathbf{v} := \mathbf{n} \cdot \mathbf{curl} \tilde{\mathbf{v}}, \\ \text{surface divergence : } & \mathbf{div}_\Gamma \mathbf{v} := \mathbf{div} \tilde{\mathbf{v}} - D\tilde{\mathbf{v}}\mathbf{n} \cdot \mathbf{n}. \end{aligned}$$

Note that these differential operators are related to the exterior derivative  $\mathbf{d}_\Gamma$  on  $\Gamma$ , see Table 5.3.

**5.2. Impedance and Neumann BVPs.** We recast the right-hand-side functional of (4.14)

$$\begin{aligned} \ell(\boldsymbol{\eta}) := & - \int_\Gamma \text{Tr } i_{\mathbf{v}} (*_\alpha \mathbf{d}\boldsymbol{\omega} \wedge \mathbf{d}\boldsymbol{\eta} - *_\kappa \boldsymbol{\omega} \wedge \boldsymbol{\eta}) - \\ & i\lambda \int_\Gamma \text{Tr } i_{\mathbf{v}} \mathbf{d}(i_{\mathbf{n}}(*\boldsymbol{\omega}) \wedge \boldsymbol{\eta}) - i\lambda \int_\Gamma \text{Tr}(i_{\delta\mathbf{n}}(*\boldsymbol{\omega}) \wedge \boldsymbol{\eta}), \end{aligned}$$

found in Theorem 4.4 and the boundary condition

$$\begin{aligned} T(\boldsymbol{\omega}) = & (-1)^l \mathbf{d}_\Gamma \{(\mathbf{v} \cdot \mathbf{n}) \alpha *_\Gamma \mathbf{d}_\Gamma \text{Tr } \boldsymbol{\omega}\} + \\ & (\mathbf{v} \cdot \mathbf{n}) \left\{ \kappa *_\Gamma \text{Tr } \boldsymbol{\omega} - i\lambda \text{Tr}(i_{\mathbf{n}}(\mathbf{d}(i_{\mathbf{n}}(*\boldsymbol{\omega})))) \right\} - i\lambda \text{Tr}(i_{\delta\mathbf{n}}(*\boldsymbol{\omega})), \end{aligned}$$

from (4.19) as equivalent vector calculus expressions depending on the order  $l$  of the differential form  $\boldsymbol{\omega}$ . We rely on the expression (4.13) for the tangential vector field  $\delta\mathbf{n}$ .

**For  $l = 0$**  (acoustic scattering) we use function proxies  $u, v$  for the forms  $\boldsymbol{\omega}$  and  $\boldsymbol{\eta}$  and note that the exterior derivatives  $\mathbf{d}$  in the functional  $\ell$  act on 0-forms and 2-forms, respectively. We observe that  $\text{Tr } i_{\delta\mathbf{n}} * \boldsymbol{\omega} = 0$  in this case, since  $*\boldsymbol{\omega}$  is a 3-form. Thus we get

$$\ell(v) = - \int_\Gamma (\mathbf{v} \cdot \mathbf{n}) (\alpha \mathbf{grad} u \cdot \mathbf{grad} v - \kappa uv - i\lambda \mathbf{div}(\mathbf{n}uv)) \, dS + \quad (5.1)$$

$$i\lambda \int_\Gamma \underbrace{\mathbf{grad}_\Gamma(\mathbf{v} \cdot \mathbf{n}) uv \cdot \mathbf{n}}_{=0} \, dS, \quad (5.2)$$

$$\begin{aligned} T(u) &= \mathbf{div}_\Gamma((\mathbf{v} \cdot \mathbf{n}) \alpha \mathbf{grad}_\Gamma u) + (\mathbf{v} \cdot \mathbf{n}) (\kappa u - i\lambda \mathbf{div}(u\mathbf{n})) \\ &= \mathbf{div}_\Gamma(\alpha (\mathbf{v} \cdot \mathbf{n}) \mathbf{grad}_\Gamma u) + \kappa u (\mathbf{v} \cdot \mathbf{n}) - i\lambda (\mathbf{v} \cdot \mathbf{n}) \frac{\partial u}{\partial \mathbf{n}} - i\lambda (\mathbf{v} \cdot \mathbf{n}) \mathfrak{H}u. \end{aligned} \quad (5.3)$$

The last formula is a consequence of the product rule and  $\mathbf{div} \mathbf{n} = \mathfrak{H}$ , where  $\mathfrak{H}$  is the additive mean curvature.

Shape derivatives for solutions of acoustic impedance boundary value problems were first presented by F. Hettlich in [14, Theorem 2.1], later corrected in [15]. Note that the impedance case covers the Neumann one [28, Theorem 3.2] for  $\lambda = 0$ .

**For  $l = 1$**  (electromagnetic scattering) the vector proxies of  $\boldsymbol{\omega}$  and  $\boldsymbol{\eta}$  are vector-valued functions  $\mathbf{E}$  and  $\mathbf{F}$ . Appealing to Table 5.3 and surface Hodge operators like (3.3) we find

$$\ell(\mathbf{F}) = - \int_\Gamma (\mathbf{v} \cdot \mathbf{n}) (\alpha \mathbf{curl} \mathbf{E} \cdot \mathbf{curl} \mathbf{F} - \kappa \mathbf{E} \cdot \mathbf{F} - i\lambda \mathbf{div}((\mathbf{E} \times \mathbf{n}) \times \mathbf{F})) \, dS - \quad (5.4)$$

$$i\lambda \int_\Gamma (\mathbf{v} \cdot \mathbf{n}) \mathbf{E} \times \mathbf{grad}_\Gamma(\mathbf{v} \cdot \mathbf{n}) \cdot \mathbf{F} \, dS, \quad (5.5)$$

$$\begin{aligned} T(\mathbf{E}) &= - \mathbf{grad}_\Gamma((\mathbf{v} \cdot \mathbf{n}) \alpha \mathbf{curl}_\Gamma \mathbf{E}) + (\mathbf{v} \cdot \mathbf{n}) (\kappa(\mathbf{E} \times \mathbf{n}) - i\lambda(\mathbf{n} \times \mathbf{curl}(\mathbf{E} \times \mathbf{n}))) \\ &\quad - i\lambda (\mathbf{v} \cdot \mathbf{n}) \mathbf{E} \times \mathbf{grad}_\Gamma(\mathbf{v} \cdot \mathbf{n}), \\ &= - \mathbf{grad}_\Gamma((\mathbf{v} \cdot \mathbf{n}) \alpha \mathbf{curl}_\Gamma \mathbf{E}_T) + (\mathbf{v} \cdot \mathbf{n}) \kappa(\mathbf{E} \times \mathbf{n}) \\ &\quad - i\lambda (\mathbf{v} \cdot \mathbf{n}) \mathbf{E} \times \mathbf{grad}_\Gamma(\mathbf{v} \cdot \mathbf{n}), \end{aligned} \quad (5.6)$$

$$-i\lambda(\mathbf{v} \cdot \mathbf{n}) \mathbf{n} \times S(\mathbf{E}) - i\lambda(\mathbf{v} \cdot \mathbf{n}) \left( \mathbf{n} \times \frac{\partial}{\partial \mathbf{n}} \mathbf{E} \right) + i\lambda(\mathbf{v} \cdot \mathbf{n}) \mathfrak{H}(\mathbf{n} \times \mathbf{E}) . \quad (5.7)$$

We owe the last identity to the product rule and the formula  $\mathbf{div} \mathbf{n} = \mathfrak{H}$ :

$$\begin{aligned} \mathbf{curl}(\mathbf{E} \times \mathbf{n}) &= \mathbf{E}(\mathbf{div} \mathbf{n}) - \mathbf{n}(\mathbf{div} \mathbf{E}) + (\mathbf{n} \cdot \nabla) \mathbf{E} - (\mathbf{E} \cdot \nabla) \mathbf{n} \\ &= \mathfrak{H} \mathbf{E} + \frac{\partial}{\partial \mathbf{n}} \mathbf{E} - S(\mathbf{E}) \quad \text{on } \Gamma , \end{aligned} \quad (5.8)$$

where we used the assumption that there is no electric charge density, namely  $\mathbf{div} \mathbf{E} = 0$ .  $S = \nabla \mathbf{n}$  is the Weingarten map, namely the second fundamental form of the boundary  $\Gamma$  pointing to the exterior.

Shape derivatives in the context of electromagnetic impedance boundary value problems were first studied by Haddar and Kress in [10, Theorem 3.4] using the boundary integral equation method. The result obtained in (5.5) matches that of [10, Eq. 3.18] when converting the latter to a form involving only the electric field  $\mathbf{E}$ .

It is pointed out that the PEC and PMC conditions should be symmetric to each other by noticing the symmetry of  $(\mathbf{E}, \mathbf{H})$  and  $(\mathbf{H}, -\mathbf{E})$  since both of them satisfy Maxwell's system.

**5.3. Dirichlet BVPs.** We recast the right-hand-side functional of (4.21)

$$\ell \left( \begin{pmatrix} \boldsymbol{\tau} \\ \boldsymbol{\nu} \end{pmatrix} \right) := -(-1)^{(l+1)(d-1)} \int_{\Gamma} \text{Tr}(i_{\mathbf{v}} \mathbf{d}\boldsymbol{\omega}) \wedge \boldsymbol{\tau} + (-1)^l \int_{\Gamma} \text{Tr}(i_{\mathbf{v}} \boldsymbol{\omega}) \wedge \mathbf{d}\boldsymbol{\tau}$$

found in Theorem 4.6 and the boundary condition

$$G(\boldsymbol{\omega}) := (\mathbf{v} \cdot \mathbf{n}) \text{Tr}(i_{\mathbf{n}} \mathbf{d}\boldsymbol{\omega}) - \mathbf{d}_{\Gamma} \{ (\mathbf{v} \cdot \mathbf{n}) \text{Tr}(i_{\mathbf{n}} \boldsymbol{\omega}) \} .$$

from (4.22) as equivalent vector calculus expressions depending on the order  $l$  of the differential form  $\boldsymbol{\omega}$ .

**For  $l = 0$**  (acoustic scattering) we use function proxies  $u$ ,  $\mathbf{w}$  and  $v$ , respectively, for the forms  $\boldsymbol{\omega}$ ,  $\boldsymbol{\tau}$  and  $\boldsymbol{\nu}$  and note that the exterior derivatives  $\mathbf{d}$  in then functional  $\ell$  act on 0-forms and 2-forms, respectively. Thus, due to  $i_{\mathbf{n}} \boldsymbol{\omega} = 0$  we arrive at

$$\ell \left( \begin{pmatrix} \mathbf{w} \\ v \end{pmatrix} \right) = - \int_{\Gamma} (\mathbf{v} \cdot \mathbf{n}) (\mathbf{grad} u \cdot \mathbf{n}) \mathbf{w} \cdot \mathbf{d}S , \quad (5.9)$$

$$G(u) = - (\mathbf{v} \cdot \mathbf{n}) \frac{\partial u}{\partial \mathbf{n}} . \quad (5.10)$$

The first expressions for the shape derivatives for acoustic scattering problems with Dirichlet boundary conditions can be found in [24, Theorem 2.1] proved via variational formulation.

**For  $l = 1$**  (electromagnetic scattering) the vector proxies  $\mathbf{E}$ ,  $\mathbf{B}$  and  $\mathbf{F}$  are used respectively for the forms  $\boldsymbol{\omega}$ ,  $\boldsymbol{\tau}$  and  $\boldsymbol{\nu}$ . Appealing to Table 5.3 we find

$$\ell \left( \begin{pmatrix} \mathbf{B} \\ \mathbf{F} \end{pmatrix} \right) = - \int_{\Gamma} (\mathbf{v} \cdot \mathbf{n}) (\mathbf{curl} \mathbf{E} \times \mathbf{n}) \cdot \mathbf{B} - (\mathbf{v} \cdot \mathbf{n}) (\mathbf{E} \cdot \mathbf{n}) \mathbf{div} \mathbf{B} \, \mathbf{d}S , \quad (5.11)$$

$$G(\mathbf{E}) = - (\mathbf{v} \cdot \mathbf{n}) (\mathbf{curl} \mathbf{E} \times \mathbf{n}) - \mathbf{grad}_{\Gamma} ((\mathbf{v} \cdot \mathbf{n}) (\mathbf{n} \cdot \mathbf{E})) . \quad (5.12)$$

We apply the surface Green's identity from (5.11) to (5.12). The electromagnetic obstacle scattering problem with perfect electric conductor (PEC) condition was first addressed by R. Potthast [33, Theorem 7] via the BIE approach, and was later studied by R. Kress [27, Theorem 10.1]. All these existing results hold only for isotropic homogeneous electric and magnetic parameters.

**5.4. Transmission problems.** We recast the right-hand-side functional of (4.21)

$$\begin{aligned} \ell \left( \begin{pmatrix} \boldsymbol{\eta} \\ \boldsymbol{\mu} \end{pmatrix} \right) &:= - \int_{\Gamma} \text{Tr } i_{\mathbf{v}} ([[*_{\alpha} \mathbf{d} \boldsymbol{\omega}]]_{\Gamma} \wedge \mathbf{d} \boldsymbol{\eta} - [*_{\kappa} \boldsymbol{\omega}]_{\Gamma} \wedge \boldsymbol{\eta}) + \\ &\quad \text{Tr}(i_{\mathbf{v}} \mathbf{d} [\boldsymbol{\omega}]_{\Gamma}) \wedge \boldsymbol{\mu} + \mathbf{d}_{\Gamma} \text{Tr}(i_{\mathbf{v}} [\boldsymbol{\omega}]_{\Gamma}) \wedge \boldsymbol{\mu}. \end{aligned}$$

found in Theorem 4.7 and the interface jump data

$$\begin{aligned} G_1(\boldsymbol{\omega}) &:= -(\mathbf{v} \cdot \mathbf{n}) \text{Tr}(i_{\mathbf{n}} \mathbf{d} [\boldsymbol{\omega}]_{\Gamma}) - \mathbf{d}_{\Gamma} \{(\mathbf{v} \cdot \mathbf{n}) i_{\mathbf{n}} [\boldsymbol{\omega}]_{\Gamma}\}, \\ G_2(\boldsymbol{\omega}) &:= (-1)^{d-l-1} \mathbf{d}_{\Gamma} \{(\mathbf{v} \cdot \mathbf{n}) [\text{Tr } i_{\mathbf{n}} *_{\alpha} \mathbf{d} \boldsymbol{\omega}]_{\Gamma}\} + (\mathbf{v} \cdot \mathbf{n}) [\text{Tr } i_{\mathbf{n}} *_{\kappa} \boldsymbol{\omega}]_{\Gamma}. \end{aligned}$$

from (4.26) and (4.29) as equivalent vector calculus expressions depending on the order  $l$  of the differential form  $\boldsymbol{\omega}$ .

**For  $l = 0$**  (acoustic scattering) we use function proxies  $u, v$  and  $\nu$ , respectively, for the forms  $\boldsymbol{\omega}, \boldsymbol{\eta}$  and  $\boldsymbol{\nu}$ . Thanks to  $i_{\mathbf{n}} \boldsymbol{\omega} = 0$  we obtain

$$\begin{aligned} \ell \left( \begin{pmatrix} v \\ \nu \end{pmatrix} \right) &= - \int_{\Gamma} (\mathbf{v} \cdot \mathbf{n}) ([\alpha \mathbf{grad} u] \cdot \mathbf{grad} v - [\kappa u] \nu) \\ &\quad + (\mathbf{v} \cdot \mathbf{n}) (\mathbf{n} \cdot \mathbf{grad}[u]) \nu \, dS, \end{aligned} \quad (5.13)$$

$$G_1(u) = -(\mathbf{v} \cdot \mathbf{n}) \left[ \frac{\partial u}{\partial \mathbf{n}} \right]. \quad (5.14)$$

$$G_2(u) = \mathbf{div}_{\Gamma}([\alpha] (\mathbf{v} \cdot \mathbf{n}) \mathbf{grad}_{\Gamma} u) + (\mathbf{v} \cdot \mathbf{n}) [\kappa] u. \quad (5.15)$$

$$(5.16)$$

These formulas were first obtained by F. Hettlich [14, Theorem 3.2] via the variational approach. By means of the BIE method, the transmission case was also successfully solved by T. Hohage and C. Schormann [22, Theorem 4.2] in two dimensions.

**For  $l = 1$**  (electromagnetic scattering) we use vector proxies  $\mathbf{E}, \mathbf{F}$  and  $\mathbf{V}$  for the forms  $\boldsymbol{\omega}, \boldsymbol{\eta}$  and  $\boldsymbol{\nu}$ , respectively. Appealing to Table 5.3 we find

$$\ell \left( \begin{pmatrix} \mathbf{F} \\ \mathbf{V} \end{pmatrix} \right) = - \int_{\Gamma} (\mathbf{v} \cdot \mathbf{n}) ([\alpha \mathbf{curl} \mathbf{E}] \cdot \mathbf{curl} \mathbf{F} - [\kappa \mathbf{E}] \cdot \mathbf{F}) \quad (5.17)$$

$$- i\lambda \mathbf{div}((\mathbf{E} \times \mathbf{n}) \times \mathbf{F})) \, dS \quad (5.18)$$

$$- \int_{\Gamma} (\mathbf{v} \cdot \mathbf{n}) (\mathbf{n} \times \mathbf{curl} \mathbf{E}) \cdot \mathbf{V} - \mathbf{grad}_{\Gamma}((\mathbf{v} \cdot \mathbf{n}) (\mathbf{E} \cdot \mathbf{n})) \cdot \mathbf{V} \, dS, \quad (5.19)$$

$$G_1(\mathbf{E}) = - \mathbf{grad}_{\Gamma}((\mathbf{v} \cdot \mathbf{n}) [\mathbf{n} \cdot \mathbf{E}]) - (\mathbf{v} \cdot \mathbf{n}) [\mathbf{curl} \mathbf{E} \times \mathbf{n}]. \quad (5.20)$$

$$G_2(\mathbf{E}) = - \mathbf{grad}_{\Gamma}((\mathbf{v} \cdot \mathbf{n}) [\alpha \mathbf{curl}_{\Gamma} \mathbf{E}]) + \mathbf{v} \cdot \mathbf{n} [\kappa] \mathbf{E} \times \mathbf{n} \quad (5.21)$$

Shape derivatives for electromagnetic transmission problems were successfully tackled by M. Costabel and F. Le Louër [6, Theorem 6.6] via the BIE approach. Their result covers media with discontinuity only in the magnetic permeability. The results can also be found in [16, Theorem 4.1] there obtained by the variational approach.

Finally, in Tables 5.6 and 5.7 we summarize the boundary value problems and transmission problems satisfied by the shape derivatives of the solutions to acoustic and electromagnetic scattering problems *in strong form*. Note that in some cases listed in Table 5.7 a rotation by 90 degrees through taking the cross product with the exterior unit normal  $\mathbf{n}$  has to be applied to recover formulas given above.

Table 5.6: Shape derivatives of acoustic scattering problems.

PDE	Obstacle scattering	$-\mathbf{div}(\alpha \mathbf{grad} \delta u) - \kappa \delta u = 0$ in $\Omega^e$
	Medium scattering	$\begin{cases} -\mathbf{div}(\alpha_i \mathbf{grad} \delta u) - \kappa_i \delta u = 0 & \text{in } \Omega \\ -\mathbf{div}(\alpha_e \mathbf{grad} \delta u) - \kappa_e \delta u = 0 & \text{in } \Omega^e \end{cases}$
BC /IC on $\Gamma$	Sound-soft	$\delta u = -(\mathbf{v} \cdot \mathbf{n}) \frac{\partial u}{\partial \mathbf{n}}$
	Sound-hard	$\alpha \frac{\partial \delta u}{\partial \mathbf{n}} = \mathbf{div}_\Gamma(\alpha (\mathbf{v} \cdot \mathbf{n}) \mathbf{grad}_\Gamma u) + \kappa u (\mathbf{v} \cdot \mathbf{n})$
	Impedance	$\begin{cases} \alpha \frac{\partial \delta u}{\partial \mathbf{n}} \\ +i\lambda \delta u \end{cases} = \begin{cases} \mathbf{div}_\Gamma(\alpha (\mathbf{v} \cdot \mathbf{n}) \mathbf{grad}_\Gamma u) + \kappa u (\mathbf{v} \cdot \mathbf{n}) \\ -i\lambda (\mathbf{v} \cdot \mathbf{n}) \frac{\partial u}{\partial \mathbf{n}} \\ -i\lambda (\mathbf{v} \cdot \mathbf{n}) \mathcal{H}u \end{cases}$
	Transmission	$\begin{cases} [\delta u] \\ [\alpha \frac{\partial \delta u}{\partial \mathbf{n}}] \end{cases} = \begin{cases} -(\mathbf{v} \cdot \mathbf{n}) [\frac{\partial u}{\partial \mathbf{n}}] \\ \mathbf{div}_\Gamma([\alpha] (\mathbf{v} \cdot \mathbf{n}) \mathbf{grad}_\Gamma u) + (\mathbf{v} \cdot \mathbf{n}) [\kappa] u \end{cases}$

**6. Conclusion.** Harnessing exterior calculus we have accomplished a unified characterization of shape derivatives of solutions of a wide array second-order boundary value problems in variational form. Acoustic and electromagnetic scattering problems are covered as important special cases. Our approach naturally accommodates variable coefficients.

Though shape optimization can avoid the use of shape derivatives [17, Section 1.6.2], they are indispensable for linearization-based shape uncertainty quantification [11, 12, 23]. In this area we see the main relevance of our results.

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#### Appendix A. Proof of Eq. (3.3).

LEMMA A.1. *If  $\lambda$  is a Riemannian metric on  $\Omega \subset \mathbb{R}^d$ ,  $\Gamma \subset \Omega$  an oriented,  $d-1$ -dimensional  $C^1$ -submanifold, then,*

$$*_\lambda^\Gamma \text{Tr}(\omega) = \text{Tr}(i_{\mathbf{n}} *_\lambda \omega) \quad \text{for all } \omega \in C^0(\wedge^l(\overline{\Omega}_R)), \quad 0 \leq l < d,$$

where  $*_\lambda$  is the Hodge operator associated with  $\lambda$ ,  $*_\lambda^\Gamma$  that on  $\Gamma$  induced by the restriction of  $\lambda$  to  $\Gamma$ , and  $\mathbf{n}$  stands for the unit normal (w.r.t.  $\lambda$ ) on  $\Gamma$ .

*Proof.* Fix  $\mathbf{x} \in \Gamma$  and a smooth  $l$ -form  $\omega \in \mathcal{DF}^{l,\infty}(\overline{\Omega})$ . Pick a positively oriented  $\lambda$ -orthonormal frame  $\{\mathbf{t}_1, \dots, \mathbf{t}_{d-1}\}$  of the tangent space to  $\Gamma$  in  $\mathbf{x}$ . Then  $\{\mathbf{n}, \mathbf{t}_1, \dots, \mathbf{t}_{d-1}\}$  will be a positively oriented  $\lambda$ -orthonormal basis for  $\mathbb{R}^d$ .

Let  $J = (j_1, \dots, j_{d-1-l})$  be an  $d-1-l$ -tuple of pairwise distance numbers  $\in \{1, \dots, d-1\}$ , and  $K = (k_1, \dots, k_l)$  an  $l$ -tuple from the same set such that the concatenation  $(J, K)$  yields a positive permutation of  $\{1, \dots, d-1\}$ . By the definition of  $*_\lambda^\Gamma$  we have

$$*_\lambda^\Gamma \text{Tr}(\omega)(\mathbf{x})(\mathbf{t}_{j_1}, \dots, \mathbf{t}_{j_{d-1-l}}) = \omega(\mathbf{x})(\mathbf{t}_{k_1}, \dots, \mathbf{t}_{k_l}).$$

Table 5.7: Shape derivatives of electromagnetic scattering problems. We give different versions of PEC boundary conditions differing by in-plane rotations on  $\Gamma$ . (IBC *hat*= impedance boundary value problem, TP  $\hat{=}$  transmission problem)

PDE	Obstacle scattering	$\mathbf{curl}(\alpha \mathbf{curl} \delta \mathbf{E}) - \kappa \delta \mathbf{E} = 0 \quad \text{in } \Omega^e$
	Medium scattering	$\begin{cases} \mathbf{curl}(\alpha_i \mathbf{curl} \delta \mathbf{E}) - \kappa_i \delta \mathbf{E} = 0 & \text{in } \Omega \\ \mathbf{curl}(\alpha_e \mathbf{curl} \delta \mathbf{E}) - \kappa_e \delta \mathbf{E} = 0 & \text{in } \Omega^e \end{cases}$
BC /IC on $\Gamma$	PEC	$\mathbf{n} \times \delta \mathbf{E} = \begin{cases} \mathbf{curl}_\Gamma((\mathbf{v} \cdot \mathbf{n})(\mathbf{n} \cdot \mathbf{E})) \\ -(\mathbf{v} \cdot \mathbf{n})(\mathbf{n} \times \mathbf{curl} \mathbf{E}) \times \mathbf{n} \end{cases}$
	PEC**	$\mathbf{n} \times \delta \mathbf{E} = \begin{cases} -\mathbf{n} \times \mathbf{grad}_\Gamma((\mathbf{v} \cdot \mathbf{n})(\mathbf{n} \cdot \mathbf{E})) \\ -(\mathbf{v} \cdot \mathbf{n})\mathbf{n} \times (\mathbf{curl} \mathbf{E} \times \mathbf{n}) \end{cases}$
	PEC*	$\delta \mathbf{E}_T = (\mathbf{n} \times \delta \mathbf{E}) \times \mathbf{n} = \begin{cases} -\mathbf{grad}_\Gamma((\mathbf{v} \cdot \mathbf{n})(\mathbf{n} \cdot \mathbf{E})) \\ -(\mathbf{v} \cdot \mathbf{n})(\mathbf{curl} \mathbf{E} \times \mathbf{n}) \end{cases}$
	PEC <sup>†</sup>	$\delta \mathbf{E}_T = (\mathbf{n} \times \delta \mathbf{E}) \times \mathbf{n} = \begin{cases} -(\mathbf{E} \cdot \mathbf{n}) \mathbf{grad}_\Gamma(\mathbf{v} \cdot \mathbf{n}) \\ -(\mathbf{v} \cdot \mathbf{n}) \left( \frac{\partial}{\partial \mathbf{n}} \mathbf{E}_T - S(\mathbf{E}) \right) \end{cases}$
	PMC	$\alpha \mathbf{n} \times (\mathbf{curl} \delta \mathbf{E}) = \begin{cases} \mathbf{curl}_\Gamma((\mathbf{v} \cdot \mathbf{n}) \alpha \mathbf{curl}_\Gamma \mathbf{E}_T) \\ +(\mathbf{v} \cdot \mathbf{n}) \kappa \mathbf{E}_T \end{cases}$
	IBC	$\begin{cases} \alpha \mathbf{n} \times (\mathbf{curl} \delta \mathbf{E}) \\ -i\lambda \delta \mathbf{E}_T \end{cases} = \begin{cases} \mathbf{curl}_\Gamma((\mathbf{v} \cdot \mathbf{n}) \alpha \mathbf{curl}_\Gamma \mathbf{E}_T) \\ +(\mathbf{v} \cdot \mathbf{n}) \kappa \mathbf{E}_T \\ +i\lambda((\mathbf{E} \cdot \mathbf{n}) \mathbf{grad}_\Gamma(\mathbf{v} \cdot \mathbf{n}) \\ +(\mathbf{v} \cdot \mathbf{n}) \left( \frac{\partial}{\partial \mathbf{n}} \mathbf{E}_T - S(\mathbf{E}) \right)) \\ +i\lambda(\mathbf{v} \cdot \mathbf{n}) \mathfrak{H} \mathbf{E}_T \end{cases}$
TP	$\begin{cases} [\mathbf{n} \times \delta \mathbf{E}] \\ [\alpha \mathbf{n} \times (\mathbf{curl} \delta \mathbf{E})] \end{cases} = \begin{cases} \mathbf{curl}_\Gamma((\mathbf{v} \cdot \mathbf{n}) [\mathbf{n} \cdot \mathbf{E}]) \\ -(\mathbf{v} \cdot \mathbf{n}) ([\mathbf{n} \times \mathbf{curl} \mathbf{E}] ) \times \mathbf{n} \\ \mathbf{curl}_\Gamma((\mathbf{v} \cdot \mathbf{n}) [\alpha \mathbf{curl}_\Gamma \mathbf{E}]) \\ +\mathbf{v} \cdot \mathbf{n} [\kappa] \mathbf{E}_T \end{cases}$	

Appealing to the definition of the Hodge operator in the volume, we obtain the same expression, because  $(\mathbf{t}_{j_1}, \dots, \mathbf{t}_{d-1-l}, \mathbf{t}_{k_1}, \dots, \mathbf{t}_l)$  is a positive  $\lambda$ -orthonormal basis of  $\mathbb{R}^d$ :

$$\text{Tr}(i_{\mathbf{n}} *_{\lambda} \omega)(\mathbf{x})(\mathbf{t}_{j_1}, \dots, \mathbf{t}_{j_{d-1-l}}) = (*_{\lambda} \omega)(\mathbf{x})(\mathbf{n}, \mathbf{t}_{j_1}, \dots, \mathbf{t}_{j_{d-1-l}}) = \omega(\mathbf{x})(\mathbf{t}_{k_1}, \dots, \mathbf{t}_{k_l}).$$

□

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