Reconstructing the Shape and Measuring Chirality of Obstacles in Electromagnetic Scattering

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1. Introduction

The main theme in this thesis is, as the title suggests, electromagnetic scattering. The behaviour of electromagnetic waves is described by Maxwell's equations. We will consider solutions, which are periodic in time. Therefore, Maxwell's equations reduce to a coupled system of partial differential equations with the two unknowns being the vector fields E and H, the electric and magnetic field. A general electromagnetic scattering problem is depicted in

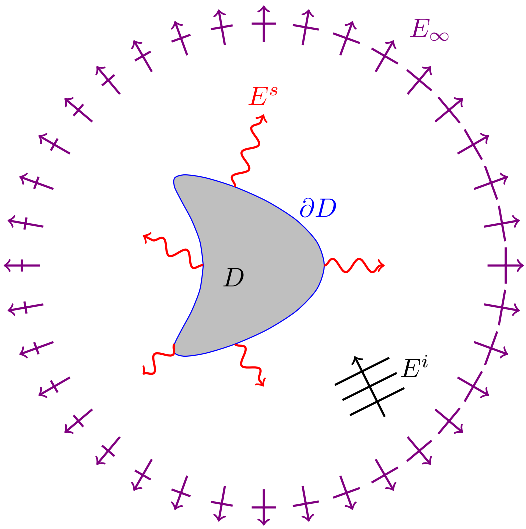

Figure 1.1: Sketch of a scattering problem.

Figure 1.1. In the presence of an incident field E^i, a scatterer D gives rise to a scattered field E^s. This is described by boundary or transmission conditions defined for the total field $E = E^s + E^i$ on the boundary ∂D of the scatterer. The scattered field decays as the distance from the scatterer grows due to a radiation condition. One can consider an expansion of the scattered field with respect to how fast the solution is decaying. The leading order term with the slowest decay is called far field pattern E_∞.

Section 2 is centered around the well known mathematical treatment of several scattering problems and serves as an introduction to electromagnetic scattering problems (see Section 2.1). We will introduce appropriate Sobolev spaces (see Section 2.2) and present suitable weak formulations (see Section 2.4).

Section 3 is concerned with the following question: How do solutions of electromagnetic scattering problems behave with respect to perturbations of the boundary ∂D? We will show, that solutions of several scattering problems are differentiable with respect to the boundary. For the simplest case, the perfect conductor, we will also show, that the solutions are twice differentiable. As it turns out, the derivative of the far field pattern with respect to variations of the boundary only depends on the *domain derivative*, which is a solution to the scattering problem at hand with different inhomogeneous boundary condition. We will provide a characterization of the domain derivative for each considered scattering problem. A characterization of the second domain derivative of the perfect conductor is also presented. Our chosen approach relies heavily on the mathematical framework presented in Section 2.

In Section 4, we present an approach to actually reconstruct the shape of a scattering object. We employ an iterative regularized Newton scheme to solve the following, inverse problem: Given a far field pattern E_∞ with respect to one incident wave, how can we determine the shape ∂D of our scatterer? We will show in detail, how one can set up such a scheme for the class of star shaped domains with appropriate regularization. Since the scheme does not depend on a specific scattering problem, it can be applied to every setting from Section 2.1.

The interaction of the electric and magnetic field with the surrounding medium is described by constitutive relations. Most materials, for example vacuum, can be described by linear material laws with scalar coefficients. Often more complex material laws are considered to model optical active media. One example of optical activity is *chirality*. Considering incident fields of purely one helicity, one can ask the following question: Can we obtain the response of the scatterer with respect to incident fields of the opposite helicity by considering a rotated and mirrored image of the original scatterer? If the answer is no, a scatterer is called chiral. Considering two chiral scatterer, the following question arises: Which of these scatterer is *more* chiral?

In Section 5, we consider a new definition of chirality, proposed in [18]. They define a measure of chirality which gives an answer to the question, how chiral a scatterer is and potentially can be. We investigate this new measure of chirality in the context of time-harmonic electromagnetic scattering. In order to find scattering objects with high measure of chirality, one might think of using a gradient type optimization scheme. It seems that the measure of chirality lacks the necessary regularity. We will therefore propose a slightly modified measure of chirality, prove its higher regularity and investigate its relation to the original measure of chirality.

In Section 6 we provide numerous numerical examples to illustrate the previous sections by using and extending the open source boundary element method library BEMPP (`https://bempp.com/`), which provides the necessary implementations of boundary element spaces, potentials and boundary operators. We present integral formulations for the scattering problems, which can also be used to calculate domain derivatives. The boundary conditions that characterize the domain derivatives involve traces and surface derivative operators. We will present how these can be easily implemented. We will also show several actual reconstructions, using the regularized iterative Newton scheme presented in Section 4. To illustrate Section 5, we will show numerical calculations of the measure of chirality and its modification. First, we consider a model problem, where we can find analytic expressions. Secondly, we will use again BEMPP to calculate the measure of chirality and its modification for an ensemble of perfectly conducting spheres.

Finally, we present in Appendix A in detail figures of the actual reconstructions and show convergence plots of our BEMPP extensions, whose implementations can be found in Appendix B.

2. Maxwell's equations

The mathematical foundation of our work is Maxwell's equations, a system of partial differential equations in time and space, which couples the scalar *charge density* ρ and the vector valued *electric field* $\mathcal{E}$, *electric displacement* $\mathcal{D}$, *magnetic field* $\mathcal{H}$, *magnetic flux density* $\mathcal{B}$ and *current density* $\mathcal{J}$:

$$\begin{aligned}\frac{\partial \mathcal{B}}{\partial t} + \operatorname{curl} \mathcal{E} &= 0,\\ \frac{\partial \mathcal{D}}{\partial t} - \operatorname{curl} \mathcal{H} &= -\mathcal{J},\\ \operatorname{div} \mathcal{D} &= \rho,\\ \operatorname{div} \mathcal{B} &= 0.\end{aligned}$$

In general, $\mathcal{D}$ and $\mathcal{B}$ are functions of $\mathcal{E}$ and $\mathcal{H}$. The behavior can be specified, if one makes assumptions on the media. In the following, two special cases will be considered. First, in *linear, isotropic* media, we have

$$\mathcal{D} = \varepsilon \mathcal{E}, \quad \mathcal{B} = \mu \mathcal{H}$$

with scalar *electric permittivity* ε and *magnetic permeability* μ. The second case is the *Drude-Born-Federov constitutive equations*, where

$$\mathcal{D} = \varepsilon(\mathcal{E} + \beta \operatorname{curl} \mathcal{E}), \quad \mathcal{B} = \mu(\mathcal{H} + \beta \operatorname{curl} \mathcal{H})$$

with additional scalar *chirality parameter* β. We do only consider settings without charges, i.e. $\rho = 0$. By *Ohm's law*, we have furthermore

$$\mathcal{J} = \sigma \mathcal{E}$$

with scalar *conductivity* σ. Furthermore we assume all vector fields to be periodically in time with *frequency* ω. This allows the splitting

$$\mathcal{E}(x,t) = \operatorname{Re}\left(\mathrm{e}^{-\mathrm{i}\omega t}\widehat{E}(x)\right), \quad \mathcal{H}(x,t) = \operatorname{Re}\left(\mathrm{e}^{-\mathrm{i}\omega t}\widehat{H}(x)\right),$$

with complex valued vector fields $\widehat{E}$ and $\widehat{H}$, which we will call again *electric* and *magnetic field*. Using this Ansatz, the time derivative becomes a multiplication with $-\mathrm{i}\omega$ and we arrive at the *time-harmonic Maxwell system*, which reads as

$$\operatorname{curl} \widehat{E} - \mathrm{i}\omega\mu\widehat{H} = 0, \qquad \operatorname{div} \varepsilon\widehat{E} = 0, \tag{2.0.1}$$

$$\operatorname{curl} \widehat{H} + (\mathrm{i}\omega\varepsilon - \sigma)\widehat{E} = 0, \qquad \operatorname{div} \mu\widehat{H} = 0. \tag{2.0.2}$$

for linear, isotropic media and

$$\operatorname{curl} \widehat{E} = \mathrm{i}\omega\mu(\widehat{H} + \beta \operatorname{curl} \widehat{H}), \qquad \operatorname{div}(\varepsilon(\widehat{E} + \beta \operatorname{curl} \widehat{E})) = 0, \tag{2.0.3}$$

$$\operatorname{curl} \widehat{H} = -\mathrm{i}\omega\varepsilon(\widehat{E} + \beta \operatorname{curl} \widehat{E}), \qquad \operatorname{div}(\mu(\widehat{H} + \beta \operatorname{curl} \widehat{H})) = 0 \tag{2.0.4}$$

for chiral media with $\sigma \equiv 0$. One important special case is the so called *homogeneous* medium, where all material parameters μ, ε, σ and β are constant. In this case, we can introduce the constant *wavenumber* $k \in \mathbb{C}$ defined by

$$k^2 = \omega^2 \varepsilon\mu + \mathrm{i}\omega\mu\sigma = \omega^2\mu(\varepsilon + \mathrm{i}\sigma/\omega)$$

where we choose $k > 0$ if $\sigma = 0$ and $\operatorname{Im} k > 0$ otherwise. Using the rescaling

$$E = \sqrt{\varepsilon + \mathrm{i}\sigma/\omega}\widehat{E}, \quad H = \sqrt{\mu}\widehat{H}$$

we arrive at the rescaled Maxwell system

$$\operatorname{curl} E = \mathrm{i}k\, H, \quad \operatorname{curl} H = -\mathrm{i}k\, E. \tag{2.0.5}$$

Closely connected to the Maxwell system is the Helmholtz equation

$$\Delta u + k^2 u = 0,$$

which can be derived from the *(acoustic) wave equation*

$$\frac{\partial^2 U(x,t)}{\partial t^2} = c^2 \Delta U$$

which describes the *amplitude* U of an acoustic wave in space and time with *speed of sound* c. Using again a time harmonic Ansatz $U(x,t) = \operatorname{Re}\left(\mathrm{e}^{-\mathrm{i}\omega t}u(x)\right)$, one arrives at the Helmholtz equation with *wavenumber* $k = \sqrt{\frac{c}{\omega}}$. The following Lemma illustrates the connection between the Helmholtz equation and the Maxwell system (2.0.5).

Lemma 2.1. *Let $\Omega \subset \mathbb{R}^3$ be an open set. A vector field $E \in C^2(\Omega, \mathbb{C}^3)$ combined with $H = \frac{1}{\mathrm{i}k} \operatorname{curl} E$ is a solution of the Maxwell system (2.0.5) if and only if E is a solution of*

$$\Delta E + k^2 E = 0 \quad \textit{and} \quad \operatorname{div} E = 0 \quad \textit{in } \Omega.$$

Proof. See [14, Theorem 6.4]. □

Instead of considering the Maxwell system, we can combine the two equations and consider the second order partial differential equations

$$\operatorname{curl}\operatorname{curl} E - k^2 E = 0 \quad \text{or} \quad \operatorname{curl}\operatorname{curl} H - k^2 H = 0.$$

In homogeneous media, we can easily give explicit examples of solutions of the Maxwell system. Choosing an arbitrary vector d of length one, i.e. $d \in \mathbb{R}^3$ with $|d| = 1$ and a complex vector $p \in \mathbb{C}^3$ with $d \cdot p = 0$, direct calculation shows that

$$E(x) = p\,\mathrm{e}^{\mathrm{i}kd\cdot x} \quad \text{and} \quad H(x) = (d \times p)\mathrm{e}^{\mathrm{i}kd\cdot x}$$

are solutions of the Maxwell system. The pair (E, H) is called *plane wave* with *direction* d and *polarization* p. Note that (E, H) are analytic solutions of the Maxwell system in $\mathbb{R}^3$. Another type of solutions can be generated with the help of the following Lemma.

Lemma 2.2. *Let $\Omega \subset \mathbb{R}^3$ be an open set and u a solution of $\Delta u + k^2 u = 0$ in Ω. For $p \in \mathbb{C}^3$ set*

$$E(x) = \operatorname{curl}(p\,u(x)), \quad H(x) = \frac{1}{\mathrm{i}k}\operatorname{curl} E(x).$$

The pair (E, H) is a solution of the Maxwell system in Ω.

Proof. We have $\operatorname{div} E = 0$ in Ω, since we have $\operatorname{div}\operatorname{curl} V = 0$ for any vector field $V \in C^2(\Omega, \mathbb{R}^3)$. Furthermore, we have by $\operatorname{curl}\operatorname{curl} = \nabla\operatorname{div} - \Delta$

$$-\Delta E(x) = \operatorname{curl}\operatorname{curl}\operatorname{curl}(pu(x)) = -\operatorname{curl}\Delta(pu(x)) + \operatorname{curl}\nabla\operatorname{div}(pu(x)).$$

Since $\operatorname{curl}\nabla v = 0$ for any $v \in C^2(\Omega)$, we obtain from $\Delta u + k^2 u = 0$

$$-\Delta E(x) = -\operatorname{curl}\big(p\Delta u(x)\big) = \operatorname{curl}\big(k^2 pu(x)\big) = k^2 E(x).$$

With the help of Lemma 2.1 we conclude that (E, H) is a solution of the Maxwell system. $\square$

As an example for such a solution to the Helmholtz equation, as used in Lemma 2.2, we define the analytic function u by

$$u(x) = \mathrm{e}^{\mathrm{i}kd\cdot x}$$

for some $d \in \mathbb{R}^3$ with $|d| = 1$. From

$$\frac{\partial u(x)}{\partial x_i} = \mathrm{i}k\, d_i\, u(x), \quad i = 1, 2, 3$$

we see $\Delta u + k^2 u = 0$. The function u is also called *(acoustic) plane wave* with *direction d*.

2.1. Obstacle scattering

In this section, we want to present the scattering problems, which are considered in this work. Before going into detail, let us first explain the general setting. We are always considering scatterers represented by simply connected bounded domains $D \subset \mathbb{R}^3$ which are surrounded by a homogeneous, linear, isotropic material. This could be vacuum with constant $\varepsilon_0 > 0$, $\mu_0 > 0$ and $\sigma = 0$ for instance. In the presence of a pair of incident waves (E^i, H^i), an analytic solution of the Maxwell system

$$\operatorname{curl} E - \mathrm{i}k\, H = 0, \quad \operatorname{curl} H + \mathrm{i}k\, E = 0, \tag{2.1.1}$$

with $k = \omega\sqrt{\varepsilon_0 \mu_0}$ in all of $\mathbb{R}^3$, the scatterer gives rise to a pair of scattered fields (E^s, H^s), a solution to the Maxwell system (2.1.1) in $\mathbb{R}^3 \setminus \overline{D}$. The interaction of the scatterer, which may or may not be penetrable, with the incident fields is modelled by boundary conditions on ∂D. In the case of a penetrable scatterer, we have an additional pair of fields (E, H), solutions of an Maxwell system in D, coupled by transmission conditions to (E^s, H^s) and (E^i, H^i). To enforce distinguishable behavior between the scattered and incident fields, we impose a condition at infinity, the so called *Silver-Müller radiation condition (SMRC)* which is given by

$$\lim_{|x|\to\infty} |x| \left[H^s(x) \times \frac{x}{|x|} - E^s(x) \right] = 0. \tag{2.1.2}$$

Considering a plane wave $E(x) = p\, \mathrm{e}^{\mathrm{i}kd\cdot x}$, we have

$$\begin{aligned} H(x) \times x - |x|E(x) &= \big((d \times p) \times x - |x|p\big)\mathrm{e}^{\mathrm{i}kd\cdot x} \\ &= \big((x \cdot d - |x|)p - (p \cdot x)d\big)\mathrm{e}^{\mathrm{i}kd\cdot x}. \end{aligned}$$

The factor in front of the exponential function can only vanish, if $x \cdot d = |x|$ and $p \cdot x = 0$, since $p \cdot d = 0$. This is the case, if and only if $x = d$, certainly not uniformly for $|x| \to \infty$. So plane waves do not satisfy the radiation condition. This example illustrates, how the radiation condition enforces that the scattered field behaves different than the incident field. In general, the radiation condition ensures, that the scattered fields are outgoing solutions. To be more precise, consider the solution Φ of the Helmholtz equation, given by

$$\Phi(x) = \frac{\mathrm{e}^{\pm \mathrm{i}k|x|}}{|x|},$$

which is for both signs a solution of the Helmholtz equation in $\mathbb{R}^3 \setminus \{0\}$ and describes a spherical wave. Remembering the time dependency, we arrive at the solution of the wave equation

$$U(x,t) = \mathrm{Re}\left(\frac{\mathrm{e}^{\mathrm{i}(\pm k|x| - \omega t)}}{|x|}\right).$$

Now we see, that only the function with the positive sign describes an outgoing solution. The gradient of Φ is given by

$$\nabla\Phi(x) = (\pm \mathrm{i}k)\frac{\mathrm{e}^{\pm \mathrm{i}k|x|}}{|x|}\frac{x}{|x|} - \frac{\mathrm{e}^{\pm \mathrm{i}k|x|}}{|x|^2}\frac{x}{|x|} = (\pm \mathrm{i}k)\Phi(x)\frac{x}{|x|} - \frac{\mathrm{e}^{\pm \mathrm{i}k|x|}}{|x|^2}\frac{x}{|x|}.$$

The difference between the ingoing and outgoing solution Φ is the sign of the leading term in the asymptotic behaviour of the gradient. This motivates the so called *Sommerfeld radiation condition* for acoustic scattering, given by

$$\lim_{|x|\to\infty} |x|\Big(\nabla u \cdot \frac{x}{|x|} - \mathrm{i}ku\Big) = 0. \tag{2.1.3}$$

By Lemma 2.2, we can define solutions to the Maxwell system (2.1.1) for any given $p \in \mathbb{C}^3$ by

$$E(x) = \operatorname{curl}(p\,\Phi(x)) = \nabla\Phi \times p, \quad H(x) = \frac{1}{\mathrm{i}k}\operatorname{curl} E(x), \quad x \in \mathbb{R}^3 \setminus \{0\}.$$

Calculation and recalling the time dependency leads to

$$\mathcal{E}(x,t) = \mathrm{Re}\left(\mathrm{e}^{-\mathrm{i}\omega t}E(x)\right) = \mathrm{Re}\left[\Big(\frac{x}{|x|} \times p\Big)\Big(\frac{\pm \mathrm{i}k}{|x|} - \frac{1}{|x|^2}\Big)\mathrm{e}^{\mathrm{i}(\pm k|x| - \omega t)}\right]$$

Again, we can distinguish ingoing and outgoing solutions by the sign of the slowest decaying term. The corresponding magnetic field can be calculated to be

$$\begin{aligned}
&\mathrm{i}kH(x) = \operatorname{curl} E(x) \\
&= -k^2\Phi(x)\Big(\frac{x}{|x|} \times \Big(\frac{x}{|x|} \times p\Big)\Big) + \frac{1}{|x|}\Big(\mp \mathrm{i}k + \frac{1}{|x|}\Big)\Big[3\Big(p \cdot \frac{x}{|x|}\Big)\frac{x}{|x|} - p\Big]\Phi(x).
\end{aligned}$$

If we plug this into the radiation condition (2.1.2), we arrive at

$$|x|\Big[H(x) \times \frac{x}{|x|} + E(x)\Big] = |x|\Phi(x)\Big(\frac{x}{|x|} \times p\Big)\Big[\pm \mathrm{i}k - \mathrm{i}k + \mathcal{O}\Big(\frac{1}{|x|}\Big)\Big],$$

which tends to zero for $|x| \to \infty$, if and only if we have chosen the $+$ sign in the definition of Φ, which corresponds to an outgoing field E. This is of course just a motivation, why the radiation condition makes sense. In general, the radiation condition ensures uniqueness of the solutions of the scattering problems.

We will now state the four scattering problems considered in this work in the classical form. Throughout this thesis, let $D \subset \mathbb{R}^3$ be open, bounded and simply connected.

2.1.1. Perfect conductor

For the perfect conductor, we assume D to be impenetrable, i.e. there is no electric and magnetic field inside D. The boundary value problem can then be fully stated in the unbounded domain $\mathbb{R}^3 \setminus \overline{D}$ and reads as

$$\operatorname{curl} E = \mathrm{i}k\, H, \quad \operatorname{curl} H = -\mathrm{i}k\, E \quad \text{in } \mathbb{R}^3 \setminus \overline{D}, \tag{2.1.4a}$$
$$\nu \times E = 0 \quad \text{on } \partial D, \tag{2.1.4b}$$
$$\begin{pmatrix} E^s \\ H^s \end{pmatrix} = \begin{pmatrix} E - E^i \\ H - H^i \end{pmatrix} \quad \text{satisfies SMRC}, \tag{2.1.4c}$$

where (E^i, H^i) is a solution of (2.1.1) in $\mathbb{R}^3$. Note, that the boundary condition (2.1.4b) reads as $\nu \times \widehat{E} = 0$ as well in the original scaling, since we rescaled the incident field as well.

2.1.2. Penetrable obstacle

Considering penetrable obstacles, we have an additional set of material parameters ε_D, μ_D, $\sigma_D \in \mathbb{C}$, which differ from μ_0, ε_0, i.e.

$$\begin{pmatrix} \mu_0 \\ \varepsilon_0 \end{pmatrix} \neq \begin{pmatrix} \mu_D \\ \varepsilon_D + \mathrm{i}\sigma_D/\omega \end{pmatrix}.$$

Then we have a set of Maxwell's equations in the unbounded domain $\mathbb{R}^3 \setminus \overline{D}$ as well as in the bounded domain D, which are coupled by transmission conditions. The full scattering problem then reads as

$$\operatorname{curl} E = \mathrm{i}\kappa\, H, \quad \operatorname{curl} H = -\mathrm{i}\kappa\, E \quad \text{in } D, \tag{2.1.5a}$$
$$\operatorname{curl} E = \mathrm{i}k\, H, \quad \operatorname{curl} H = -\mathrm{i}k\, E \quad \text{in } \mathbb{R}^3 \setminus \overline{D}, \tag{2.1.5b}$$
$$\frac{1}{\sqrt{\varepsilon_0}} \nu \times E\big|_+ - \frac{1}{\sqrt{\varepsilon_D + \mathrm{i}\sigma_D/\omega}} \nu \times E\big|_- = 0 \quad \text{on } \partial D, \tag{2.1.5c}$$
$$\frac{1}{\sqrt{\mu_0}} \nu \times H\big|_+ - \frac{1}{\sqrt{\mu_D}} \nu \times H\big|_- = 0 \quad \text{on } \partial D, \tag{2.1.5d}$$

$$\begin{pmatrix} E^s \\ H^s \end{pmatrix} = \begin{pmatrix} E - E^i \\ H - H^i \end{pmatrix} \quad \text{satisfies SMRC,} \tag{2.1.5e}$$

where (E^i, H^i) is a solution of (2.1.1) in $\mathbb{R}^3$ and $\kappa = \omega\sqrt{\mu_D(\varepsilon_D + \mathrm{i}\sigma_D/\omega)}$ denotes the *interior wavenumber*. Note, that the unintuitive transmission conditions (2.1.5c) and (2.1.5d) imply continuity of the tangential components of the electric and magnetic field in the original scaling

$$\nu \times \widehat{H}\big|_+ - \nu \times \widehat{H}\big|_- = 0 = \nu \times \widehat{E}\big|_+ - \nu \times \widehat{E}\big|_- .$$

2.1.3. Obstacles with impedance boundary condition

We consider again an impenetrable scatterer. On the boundary ∂D, we have an additional material parameter, the *(surface) impedance* $\lambda : \partial D \to \mathbb{R}$ which we always assume to be positive, i.e. $\lambda > 0$. Then the scattering problem with impedance boundary condition reads as

$$\operatorname{curl} E = \mathrm{i}k\, H, \quad \operatorname{curl} H = -\mathrm{i}k\, E \quad \text{in } \mathbb{R}^3 \setminus \overline{D}, \tag{2.1.6a}$$

$$\nu \times H = \lambda\big(\nu \times (E \times \nu)\big) \quad \text{on } \partial D, \tag{2.1.6b}$$

$$\begin{pmatrix} E^s \\ H^s \end{pmatrix} = \begin{pmatrix} E - E^i \\ H - H^i \end{pmatrix} \quad \text{satisfies SMRC,} \tag{2.1.6c}$$

where (E^i, H^i) is again a solution of (2.1.1) in $\mathbb{R}^3$. Note, that the boundary condition (2.1.6b) is equivalent to the impedance boundary condition

$$\nu \times \widehat{H} = \widehat{\lambda}\big(\nu \times (\widehat{E} \times \nu)\big) \quad \text{on } \partial D$$

in the original scaling with positive impedance $\widehat{\lambda} = \frac{\sqrt{\mu_0}}{\sqrt{\varepsilon_0}}\lambda > 0$.

2.1.4. Chiral media

The Maxwell system for chiral media (2.0.3) does not allow the elegant scaling. Introducing the chiral parameter $\beta > 0$ and additional $\varepsilon_D, \mu_D \in \mathbb{C}$, the scattering from chiral media reads as

$$\operatorname{curl} E = \mathrm{i}k\, H, \quad \operatorname{curl} H = -\mathrm{i}k\, E \quad \text{in } \mathbb{R}^3 \setminus \overline{D}, \tag{2.1.7a}$$

$$\operatorname{curl} E = \mathrm{i}\kappa(H + \beta \operatorname{curl} H), \quad \operatorname{curl} H = \mathrm{i}\kappa(E + \beta \operatorname{curl} E) \quad \text{in } D, \tag{2.1.7b}$$

$$\frac{1}{\sqrt{\varepsilon_0}}\nu \times E\big|_+ - \frac{1}{\sqrt{\varepsilon_D}}\nu \times E\big|_- = 0 \quad \text{on } \partial D, \tag{2.1.7c}$$

$$\frac{1}{\sqrt{\mu_0}}\nu \times H\big|_+ - \frac{1}{\sqrt{\mu_D}}\nu \times H\big|_- = 0 \quad \text{on } \partial D, \tag{2.1.7d}$$

$$\begin{pmatrix} E^s \\ H^s \end{pmatrix} = \begin{pmatrix} E - E^i \\ H - H^i \end{pmatrix} \quad \text{satisfies SMRC,} \tag{2.1.7e}$$

where (E^i, H^i) is again a solution of (2.1.7a) in $\mathbb{R}^3$ and we have the exterior and interior wavenumbers $k = \omega\sqrt{\varepsilon_0\mu_0}$ and $\kappa = \omega\sqrt{\mu_D\varepsilon_D}$, respectively. For more details and how one can derive the boundary conditions from physical laws for the various scattering cases, we refer to the detailed introduction in [33].

2.2. Sobolev spaces

In our work, we consider weak solutions of the above stated scattering problems in $H(\mathrm{curl}, \Omega)$ or in appropriate subspaces of $H(\mathrm{curl}, \Omega)$. We will briefly motivate this approach and present the necessary results. We will start by defining Sobolev spaces in Ω.

2.2.1. Sobolev spaces

We start with a partial integration formula. Let $u, v \in C^1(\overline{\Omega})$ and the boundary $\partial\Omega$ be smooth enough. Then we have

$$\int_\Omega u\nabla v \,\mathrm{d}x + \int_\Omega v\nabla u \,\mathrm{d}x = \int_{\partial\Omega} uv\nu \,\mathrm{d}s. \tag{2.2.1}$$

Motivated by this equation, we define: A function $u \in L^2(\Omega)$ is said to possess a *weak gradient* $F \in L^2(\Omega, \mathbb{C}^3)$, if

$$\int_\Omega u\nabla\varphi \,\mathrm{d}x = -\int_\Omega F\varphi \,\mathrm{d}x, \qquad \text{for all } \varphi \in C_0^\infty(\Omega).$$

Since F is unique, we use the usual notation $\nabla u = F$. We define

$$H^1(\Omega) = \{u \in L^2(\Omega) : u \text{ possesses a weak gradient in } L^2(\Omega, \mathbb{C}^3)\}.$$

This space is, together with the inner product

$$\langle u, v\rangle_{H^1(\Omega)} = \int_\Omega \left(u\overline{v} + \nabla u \cdot \overline{\nabla v}\right) \mathrm{d}x,$$

a Hilbert space. For $\varphi \in C^1(\overline{\Omega})$, one can define the *trace operator* γ by

$$\gamma\varphi = \varphi\big|_{\partial\Omega}.$$

Note that the left hand side of (2.2.1) makes sense for $u, v \in H^1(\Omega)$. By choosing the right space on the boundary $\partial\Omega$, one can extend γ to a linear bounded operator defined on $H^1(\Omega)$. This extension requires some regularity of the boundary. To be more precise the boundary $\partial\Omega$ has to be at least Lipschitz. We will present this later. Analogously, one can define Sobolev spaces of order $m \in \mathbb{N}$. For $\alpha = (\alpha_1, \alpha_2, \alpha_3)^\top \in \mathbb{N}^3$ we define the differential operator D^α by

$$D^\alpha \varphi = \frac{\partial^{\alpha_1+\alpha_2+\alpha_3}\varphi}{\partial x_1^{\alpha_1}\partial x_2^{\alpha_2}\partial x_3^{\alpha_3}}, \qquad \text{for } \varphi \in C^{\|\alpha\|}(\Omega),$$

where we define $|\alpha|$ by $|\alpha| = \alpha_1 + \alpha_2 + \alpha_3$. A function $u \in L^2(\Omega)$ is said to possess a *weak derivative f of order $\alpha \in \mathbb{N}^3$* in $L^2(\Omega)$, if there is a function $f \in L^2(\Omega)$ such that

$$\int_\Omega u D^\alpha \varphi \,\mathrm{d}x = (-1)^{|\alpha|} \int_\Omega g\varphi \,\mathrm{d}x, \qquad \text{for all } \varphi \in C_0^\infty(\Omega).$$

We use again the usual notation $D^\alpha u = g$ and define for $m \in \mathbb{N}$ the space

$$H^m(\Omega) = \{u \in L^2(\Omega) : D^\alpha u \in L^2(\Omega) \text{ for all } \alpha \in \mathbb{N}^3 \text{ with } |\alpha| \leqslant m\},$$

which is, together with the inner product

$$\langle u, v\rangle_{H^m(\Omega)} = \int_\Omega u\overline{v}\,\mathrm{d}x + \sum_{\substack{\alpha\in\mathbb{N}^3\\ \|\alpha\|\leqslant m}} \int_\Omega D^\alpha u\,\overline{D^\alpha v}\,\mathrm{d}s,$$

a Hilbert space. Considering smooth vector fields $E, V : \Omega \to \mathbb{C}^3$, we have the following partial integration formula:

$$\int_\Omega \Big(\operatorname{curl} E \cdot V - \operatorname{curl} V \cdot E\Big)\,\mathrm{d}x = \int_{\partial\Omega} (\nu \times E)\cdot(\nu \times (V \times \nu))\,\mathrm{d}s. \qquad (2.2.2)$$

Motivated by this equation, we define: A function $E \in L^2(\Omega, \mathbb{C}^3)$ is said to possess a *weak curl* $F \in L^2(\Omega, \mathbb{C}^3)$, if

$$\int_\Omega E \cdot \operatorname{curl} V\,\mathrm{d}s = \int_\Omega F \cdot V\,\mathrm{d}s \qquad \text{for all } V \in C_0^\infty(\Omega, \mathbb{C}^3).$$

We define the space $H(\operatorname{curl}, \Omega)$ as the subspace of those functions in $L^2(\Omega, \mathbb{C}^3)$ with weak curl in $L^2(\Omega, \mathbb{C}^3)$, i.e.

$$H(\operatorname{curl}, \Omega) = \{E \in L^2(\Omega, \mathbb{C}^3) :\ E \text{ possesses weak curl } F \in L^2(\Omega, \mathbb{C}^3)\}.$$

If $F \in L^2(\Omega, \mathbb{C}^3)$ is the weak curl of $E \in H(\operatorname{curl}, \Omega)$, we write again as usually $\operatorname{curl} E = F$. Together with the inner product

$$\langle E, V \rangle_{H(\operatorname{curl},\Omega)} = \langle E, V \rangle_{L^2(\Omega,\mathbb{C}^3)} + \langle \operatorname{curl} E, \operatorname{curl} V \rangle_{L^2(\Omega,\mathbb{C}^3)},$$

where $\langle A, B \rangle_{L^2(\Omega,\mathbb{C}^3)} = \int_\Omega A \cdot \overline{B}\, \mathrm{d}x$ denotes the inner product of $L^2(\Omega, \mathbb{C}^3)$, one finds that $H(\operatorname{curl}, \Omega)$ is a Hilbert space. For functions $\varphi \in C^1(\overline{\Omega}, \mathbb{C}^3)$, one can define the *tangential traces* $\gamma_t \varphi, \gamma_T \varphi$ by

$$\gamma_t \varphi = \varphi \times \nu\big|_{\partial D}, \quad \gamma_T \varphi = (\nu \times (\varphi \times \nu))\big|_{\partial D}.$$

Motivated by (2.2.2), one can extend these traces for $E \in H(\operatorname{curl}, \Omega)$, if the boundary is at least Lipschitz. We want to chose the right range space, such that γ_t and γ_T are continuous and surjective. As it turns out, we need fractional Sobolev spaces with negative index on the boundary $\partial\Omega$. We will outline, how one defines these for bounded Lipschitz domains Ω, following closely mainly [33] and also [6, 39]. For bounded domains with smooth boundaries, one could use a more elegant different approach, see e.g. [40]. But this requires some knowledge about unbounded operators on smooth manifolds. Therefore, and because above defined scattering problems can be defined and solved for bounded Lipschitz domains, we chose the more technical approach. Let us start by defining Lipschitz domains.

2.2.2. Traces and Sobolev spaces on surfaces

A bounded set $\Omega \subset \mathbb{R}^3$ is called *Lipschitz domain*, if the boundary can be locally parameterized by a Lipschitz-continuous function. That means, for every $x \in \partial\Omega$ there is an open neighborhood $\omega \subset \mathbb{R}^3$ with $x \in \omega$ satisfying the following properties. Let $B_n(p, r)$ denote the ball of radius r and center p in $\mathbb{R}^n$. Then there exists a constant $\alpha > 0$, a Lipschitz-continuous function $\psi : B_2(0, \alpha) \to [0, 1]$, a rotation $R \in \mathbb{R}^{3\times 3}$ and a translation $z \in \mathbb{R}^3$ such that the following holds

$$\begin{aligned}
\partial\Omega \cap \omega &= \{Rx + z \in \mathbb{R}^3 : (x_1, x_2) \in B_2(0, \alpha),\ x_3 = \psi(x_1, x_2)\},\\
\Omega \cap \omega &= \{Rx + z \in \mathbb{R}^3 : (x_1, x_2) \in B_2(0, \alpha),\ x_3 < \psi(x_1, x_2)\},\\
\omega \setminus \overline{D} &= \{Rx + z \in \mathbb{R}^3 : (x_1, x_2) \in B_2(0, \alpha),\ x_3 > \psi(x_1, x_2)\}.
\end{aligned}$$

We define the parametrization $\Phi : B_3(0, \alpha) \to \mathbb{R}^3$ by

$$\Phi(x) = R \begin{pmatrix} x_1 \\ x_2 \\ \psi(x_1, x_2) + x_3 \end{pmatrix} + z, \quad x \in B_3(0, \alpha).$$

Then $\Phi : B_2(0,\alpha) \times \{0\} \to \mathbb{R}^3$ is a local parametrization in ω and we have

$$\begin{aligned} \partial\Omega \cap \omega &= \{\Phi(x) : x \in B_2(0,\alpha),\, x_3 = 0\}, \\ \Omega \cap \omega &= \{\Phi(x) : x \in B_2(0,\alpha),\, x_3 < 0\}, \\ \omega \setminus \overline{\Omega} &= \{\Phi(x) : x \in B_2(0,\alpha),\, x_3 > 0\}. \end{aligned}$$

Note, that by Rademacher's theorem ψ is almost everywhere differentiable with $|\nabla\psi| \leqslant L$, where L denotes the Lipschitz constant of ψ. Some vector calculus shows

$$\left|\frac{\partial\Phi}{\partial x_1} \times \frac{\partial\Phi}{\partial x_2}\right| = \sqrt{1 + |\nabla\psi|^2}, \quad \nu(y = \Phi(x)) = \frac{1}{\sqrt{1+|\nabla\psi|^2}} R \begin{pmatrix} -\partial_{x_1}\psi(x) \\ -\partial_{x_2}\psi(x) \\ 1 \end{pmatrix}.$$

Since Ω is bounded we have that $\partial\Omega$ is compact. For every $x \in \partial\Omega$ we have such a parametrization $\Phi_x : B_2(0,\alpha_x) \to \mathbb{R}^3$ of an open neighborhood $\omega_x \subset \mathbb{R}^3$. Since $x \in \omega_x$, we have $\partial\Omega \subset \cup_{x\in\partial\Omega}\omega_x$. Since $\partial\Omega$ is compact, we can choose a finite covering $\omega_1, \ldots, \omega_N$ with $N \in \mathbb{N}$ of $\partial\Omega$, i.e. we need only N parametrizations Φ_i, $i = 1, \ldots, N$ to describe the boundary $\partial\Omega$. The boundary $\partial\Omega$ is called *of class* C^k, if we have in addition that all parametrizations ψ satisfy $\psi \in C^k$. The boundary $\partial\Omega$ is called *regular*, if $k = \infty$. In order to localize functions, we need the following theorem.

Theorem 2.3 (Partition of the Unity). *Let $K \subset \mathbb{R}^3$ be a compact set. For every finite open covering ω_i, $i = 1, \ldots, N$ with $N \in \mathbb{N}$, there exists $\lambda_i \in C^\infty(\mathbb{R}^3)$ with $\operatorname{supp}\lambda_i \subset \omega_i$ $i = 1, \ldots, N$, such that*

$$\sum_{i=1}^{N} \lambda_i(x) = 1, \qquad \textit{for all } x \in K.$$

Now let $u \in C(\partial\Omega)$. Let $\{\lambda_i\}$ be a partition of the unity with respect to the covering $\partial\Omega \subset \cup_{i=1}^N \omega_i$. Then u is represented by a sum of localized functions $v_i : B_2(0,\alpha_i) \times \{0\} \to \mathbb{C}$. First we write $u = \sum_{i=1}^N \lambda_i u$. For every function $u_i = \lambda_i u$ we can define

$$v_j(x) = u_j(\Phi_j(x)), \quad x \in B_2(0,\alpha_j) \times \{0\}.$$

We can localize the $L^2(\partial\Omega)$-norm by

$$\|u\|^2_{L^2(\partial\Omega)} = \int_{\partial\Omega} |u(y)|^2 \,\mathrm{d}s = \sum_{j=1}^{m} \int_{\partial\Omega\cap\omega_i} \lambda_j(y)|u(y)|^2 \,\mathrm{d}s$$

$$= \sum_{j=1}^{m} \int_{B_2(0,\alpha_j)} \lambda_j(\Phi_j(x))|u(\Phi_j(x))|^2 \sqrt{1 + |\nabla\psi_j(x)|^2}\,\mathrm{d}x. \quad (2.2.3)$$

From this we can see that $u \in L^2(\Omega)$ if and only if $x \mapsto \sqrt{\lambda_j(\Phi_j(x))}u(\Phi_j(x))$ is in $L^2(B_2(0,\alpha_j))$. Note that λ_i is compactly supported in ω_i and therefore v_j has compact support in $B_2(0,\alpha_j)\times\{0\}$. Thus, we can extend v_j by zero outside of $B_2(0,\alpha_j)$ to a continuous and periodic function $v_j \in C_{\mathrm{per}}([-\pi,\pi]^2)$. This localization allows us to define Sobolev spaces on the boundary by means of periodic Sobolev spaces in dimension two on some cube K with $B_2(0,\alpha_i) \subset K$. Finally, we finish the preparations of defining Sobolev spaces on the boundary by defining the space $H^s_{\mathrm{per}}(K)$, the space of periodic Sobolev functions on the cube $K = (-\pi,\pi)^2$. For $u \in L^2(K)$, the *Fourier coefficients* $u_n \in \mathbb{C}$ for $n \in \mathbb{Z}^2$ are defined as

$$u_n = \frac{1}{4\pi^2} \int_K u(x)\mathrm{e}^{-\mathrm{i}n\cdot x}\,\mathrm{d}x.$$

With these coefficients, we can define the *Fourier series* of u as the right hand side of

$$u(x) = \sum_{n\in\mathbb{Z}^2} u_n \mathrm{e}^{\mathrm{i}n\cdot x}.$$

The equality of this equation has to be understood in the $L^2(K)$ sense. A partial derivative of u is formally given by

$$\frac{\partial u}{\partial x_i} = \sum_{n\in\mathbb{Z}^2} \mathrm{i}n_i u_n \mathrm{e}^{\mathrm{i}n\cdot x}, \quad i = 1, 2.$$

Therefore we define for any real $s \geqslant 0$ the space

$$H^s_{\mathrm{per}}(K) = \{u \in L^2(K) : \sum_{n\in\mathbb{Z}^2} (1 + |n|^2)^s |u_n|^2 < \infty\},$$

which is, together with the inner product

$$\langle u, v\rangle_{H^s_{\mathrm{per}}(K)} = \sum_{n\in\mathbb{Z}^2} (1 + |n|^2)^s u_n \overline{v_n}$$

a Hilbert space. A finite sum

$$u(x) = \sum_{\substack{n\in\mathbb{Z}^2 \\ |n|\leqslant M}} u_n \mathrm{e}^{\mathrm{i}n\cdot x}, \quad x \in K, \quad u_n \in \mathbb{C}$$

is called *trigonometric polynomial.* We can also define $H^{-s}_{\text{per}}(K)$ as the completion of the space of trigonometric polynoms with respect to the norm

$$\|u\|_{H^{-s}_{\text{per}}} = \sum_n (1+|n|^2)^{-s}|u_n|^2,$$

where we sum over the finitely many Fourier coefficients u_n. We use (2.2.3) to define Sobolev spaces with non-negative exponent $s \geqslant 0$ on the boundary $\partial\Omega$ as subspaces of $L^2(\partial\Omega)$. Define the space

$$H^s(\partial D) = \{u \in L^2(\partial\Omega) : \widetilde{u_j} \in H^s_{\text{per}}(K) \text{ for all } j = 1, \dots, N\}$$

where $\widetilde{u_j}$ denotes the localization of u, i.e.

$$\widetilde{u_j}(x) = \sqrt{\lambda_j(\Phi_j(x))}\sqrt{1+|\nabla\psi_j|^2} u(\Phi_j(x)),$$

together with the associated norm

$$\|u\|^2_{H^s(\partial\Omega)} = \sum_{j=1}^{N} \|\widetilde{u_j}\|^2_{H^s_{\text{per}}(K)}.$$

The norm depends on the choice of the parametrizations and partition of the unity, but different choices lead to equivalent norms. We can also consider $H^s(\partial\Omega)$ with exponent $-s$. As it turns out, the spaces of exponents s and $-s$ are dual to each other. The dual pairing

$$_{H^{-s}(\partial\Omega)}\langle \cdot, \cdot \rangle_{H^s(\partial\Omega)} : H^{-s}(\partial\Omega) \times H^s(\partial\Omega) \to \mathbb{C}$$

is given by the extension of the $L^2(\partial\Omega)$ inner product, i.e. we have

$$_{H^{-s}(\partial\Omega)}\langle u, v \rangle_{H^s(\partial\Omega)} = \int_{\partial\Omega} u\bar{v}\,\mathrm{d}s,$$

if $u \in L^2(\partial\Omega) \cap H^{-s}(\partial\Omega)$. As it turns out, one can extend γ continuously to $H^1(\Omega)$ and the range spaces are exactly the Sobolev spaces on the boundary $H^s(\partial\Omega)$ with $s = \frac{1}{2}$. We will summarize this in the following theorem.

Theorem 2.4 (Trace theorem I)**.** *The trace operator γ can be extended to a linear bounded operator*

$$\gamma : H^1(\Omega) \to H^{\frac{1}{2}}(\partial\Omega).$$

Furthermore, γ is surjective and admits a bounded right inverse $\eta : H^{\frac{1}{2}}(\partial\Omega) \to H^1(\Omega)$, i.e.

$$u = \gamma\eta u, \qquad \textit{for all } u \in H^{\frac{1}{2}}(\partial\Omega).$$

Proof. See [33, Theorem 5.10]. □

Now we want to establish a trace theorem for functions $E \in H(\mathrm{curl}, \Omega)$. Motivated by the partial integration formula (2.2.2), the space of tangential vector fields $L^2_t(\partial\Omega)$ defined by

$$L^2_t(\partial\Omega) = \{E \in L^2(\partial\Omega, \mathbb{C}^3) : \nu \cdot E = 0 \text{ almost everywhere.}\}$$

seems to be a reasonable starting point. Analogously to the scalar case, we want to localize functions $E \in L^2_t(\partial\Omega)$. Since we want to keep the structure of tangential vector fields, we define

$$L^2_t(K) = \{E \in L^2(K, \mathbb{C}^3) : E_3 = 0 \text{ almost everywhere.}\}.$$

Now, using again a partition of the unity, we need to construct functions $\widetilde{E_i} \in L^2_t(K)$ such that we have $E \in L^2_t(\partial\Omega)$ if and only if $\widetilde{E_i} \in L^2_t(K)$ for $i = 1, \dots, N$. There are two sets of $\widetilde{E_i}$, which satisfy our needs, given by

$$\widetilde{E_i^t}(x) = \begin{cases} \sqrt{1 + |\nabla\psi_i(x)|^2}\sqrt{\lambda_i(\Phi_i(x))}F_i^{-1}(x)E(\Phi_i(x)), & x \in B_2(0, \alpha_i) \\ 0 & x \in K \setminus \overline{B_2(0, \alpha_i)} \end{cases},$$

$$\widetilde{E_i^T}(x) = \begin{cases} \sqrt{1 + |\nabla\psi_i(x)|^2}\sqrt{\lambda_i(\Phi_i(x))}F_i^{\top}(x)E(\Phi_i(x)), & x \in B_2(0, \alpha_i) \\ 0 & x \in K \setminus \overline{B_2(0, \alpha_i)} \end{cases},$$

for $x \in B_2(0, \alpha_i)$ and by 0 in $K \setminus \overline{B_2(0, \alpha_i)}$, where the matrix F_i is defined column wise by

$$F_i(x) = \left[\frac{\partial\Phi_i(x)}{\partial x_1} \middle| \frac{\partial\Phi_i(x)}{\partial x_2} \middle| \frac{\partial\Phi_i(x)}{\partial x_1} \times \frac{\partial\Phi_i(x)}{\partial x_2} \right], \quad x \in B_2(0, \alpha_i).$$

We need both sets of localized functions, since the space $H(\mathrm{curl}, \Omega)$ admits two kinds of traces, which are in different spaces. Analogously to the scalar space, we define the following vector valued periodic Sobolev spaces. We start by defining the space of *trigonometric vector polynomials* $\mathcal{T}(K, \mathbb{C}^2)$ by

$$\mathcal{T}(K, \mathbb{C}^2) = \{u \in L^2(K, \mathbb{C}^2) : u(x) = \sum_{\substack{n \in \mathbb{Z}^2 \\ |n| \leqslant M}} u_n \mathrm{e}^{\mathrm{i}n \cdot x},\ x \in K,\ u_n \in \mathbb{C}^2,\ M \in \mathbb{N}\}.$$

Next, we define two norms on $\mathcal{T}(K, \mathbb{C}^2)$ by

$$\|u\|_{H^s_{\mathrm{per}}(\mathrm{Div}, K)} = \sqrt{\sum_{n \in \mathbb{Z}^2} (1 + |n|^2)^s [|u_n|^2 + |n \cdot u_n|^2]},$$

$$\|u\|_{H^s_{\mathrm{per}}(\mathrm{Curl},K)} = \sqrt{\sum_{n\in\mathbb{Z}^2}(1+|n|^2)^s[|u_n|^2+|n\times u_n|^2]},$$

where $a\times b = a_1b_2 - a_2b_1$ for $a,b\in\mathbb{C}^2$. Then we define $H^s_{\mathrm{per}}(\mathrm{Div},K)$ and $H^s_{\mathrm{per}}(\mathrm{Curl},K)$ for any $s\in\mathbb{R}$ by the completion of $\mathcal{T}(K,\mathbb{C}^2)$ with respect to the the corresponding norm. Again, we define spaces on the boundary by localized functions. We define for $s\in\mathbb{R}$ the spaces $H^s(\mathrm{Div},\partial\Omega)$ and $H^s(\mathrm{Curl},\partial\Omega)$ as the completion of

$$\{E\in L^2_t(\partial\Omega) : \widetilde{E^t_j}\in H^s(\mathrm{Div},K),\ j=1,\dots,N\}\quad\text{and}$$
$$\{E\in L^2_t(\partial\Omega) : \widetilde{E^T_j}\in H^s(\mathrm{Curl},K),\ j=1,\dots,N\},$$

respectively, with respect to the norms

$$\|E\|_{H^s(\mathrm{Div},\partial\Omega)} = \sqrt{\sum_{j=1}^N \|\widetilde{E^t_j}\|^2_{H^s(\mathrm{Div},K)}},$$
$$\|E\|_{H^s(\mathrm{Curl},\partial\Omega)} = \sqrt{\sum_{j=1}^N \|\widetilde{E^T_j}\|^2_{H^s(\mathrm{Curl},K)}}.$$

As it turns out, one can extend γ_t and γ_T continuously to $H(\mathrm{curl},\Omega)$ and the range spaces are exactly the two spaces defined above with $s=-\frac{1}{2}$. We will summarize this in the following theorem.

Theorem 2.5 (Trace theorem II). *The trace operators γ_t and γ_T can be extended to linear bounded operators*

$$\gamma_t : H(\mathrm{curl},\Omega)\to H^{-\frac{1}{2}}(\mathrm{Div},\partial\Omega),\quad \gamma_T : H(\mathrm{curl},\Omega)\to H^{-\frac{1}{2}}(\mathrm{Curl},\partial\Omega).$$

They both have bounded right inverses η_t and η_T. Furthermore, $H^{-\frac{1}{2}}(\mathrm{Div},\partial\Omega)$ and $H^{-\frac{1}{2}}(\mathrm{Curl},\partial\Omega)$ are dual to each other, where the dual pairing

$$_{H^{-\frac{1}{2}}(\mathrm{Div},\partial\Omega)}\langle\cdot,\cdot\rangle_{H^{-\frac{1}{2}}(\mathrm{Curl},\partial\Omega)} : H^{-\frac{1}{2}}(\mathrm{Div},\partial\Omega)\times H^{-\frac{1}{2}}(\mathrm{Curl},\partial\Omega)\to\mathbb{C}$$

is given by

$$_{H^{-\frac{1}{2}}(\mathrm{Div},\partial\Omega)}\langle E,V\rangle_{H^{-\frac{1}{2}}(\mathrm{Curl},\partial\Omega)} = \int_{\partial\Omega} E\cdot\overline{V}\,\mathrm{d}s,$$

if $E\in L^2_t(\partial\Omega)\cap H^{-\frac{1}{2}}(\mathrm{Div},\partial\Omega)$ and $V\in L^2_t(\partial\Omega)\cap H^{-\frac{1}{2}}(\mathrm{Curl},\partial\Omega)$. Furthermore, we have for $E,V\in H(\mathrm{curl},\Omega)$ the partial integration formula

$$\int_\Omega \left(\overline{\mathrm{curl}\,V}\cdot E - \overline{V}\cdot\mathrm{curl}\,E\right)\mathrm{d}x = {}_{H^{-\frac{1}{2}}(\mathrm{Div},\partial\Omega)}\langle\gamma_t E,\gamma_T V\rangle_{H^{-\frac{1}{2}}(\mathrm{Curl},\partial\Omega)}. \quad (2.2.4)$$

Proof. See [33, Theorems 5.24 and 5.26]. □

2.2.3. Surface differential operators

In this section, we present several surface differential operators and their extensions to Sobolev spaces. Since we want to define these operators as classic differential operators, we assume just for this part, that Ω is a bounded domain with boundary $\partial\Omega$ of class C^2. Let $u \in C^1(\partial\Omega)$. Then we can define the *surface gradient* $\mathrm{Grad}_{\partial\Omega}$ by

$$\mathrm{Grad}_{\partial\Omega}\, u = \nabla \hat{u} - \frac{\partial \hat{u}}{\partial \nu}\nu,$$

and the *vectorial surface rotation* $\overrightarrow{\mathrm{Curl}}_{\partial\Omega}$ by

$$\overrightarrow{\mathrm{Curl}}_{\partial\Omega} u = \mathrm{Grad}_{\partial\Omega}\, u \times \nu,$$

where $\hat{u} \in C^1(U)$ denotes an arbitrary extension of u to an open set U such that $\partial\Omega \subset U$. Now let $F \in C^1(\partial\Omega, \mathbb{C}^3)$ be a tangential vector field, i.e. $F \cdot \nu = 0$ on $\partial\Omega$. Then we define the *surface divergence* $\mathrm{Div}_{\partial\Omega}$ by

$$\mathrm{Div}_{\partial\Omega}\, F = \mathrm{div}\, \hat{F} - \nu \cdot J_{\hat{F}} \nu,$$

where again $\hat{F} \in C^1(U, \mathbb{C}^3)$ denotes an extension of F to an open neighborhood U of $\partial\Omega$ and $J_{\hat{F}}$ the Jacobian of $\hat{F}$. We also define for F the *scalar surface rotation* $\mathrm{Curl}_{\partial\Omega}$ by

$$\mathrm{Curl}_{\partial\Omega}\, F = \mathrm{curl}\, \hat{F} \cdot \nu.$$

The surface gradient $\mathrm{Grad}_{\partial\Omega}$ and the surface divergence $\mathrm{Div}_{\partial\Omega}$ are coupled by duality with respect to the $L^2(\partial\Omega)$ inner product, that is we have

$$\int_{\partial\Omega} u\, \mathrm{Div}_{\partial\Omega}\, F \,\mathrm{d}s = -\int_{\partial\Omega} F \cdot \mathrm{Grad}_{\partial\Omega}\, u \,\mathrm{d}s. \tag{2.2.5}$$

The scalar surface rotation $\mathrm{Curl}_{\partial\Omega}$ can be expressed by the surface divergence $\mathrm{Div}_{\partial\Omega}$ by

$$\mathrm{Div}_{\partial\Omega}(F \times \nu) = \mathrm{Curl}_{\partial\Omega}\, F, \tag{2.2.6}$$

which could also be used as definition of $\mathrm{Curl}_{\partial\Omega}$. These operator motivate in hindsight the definition of the trace spaces $H^{-\frac{1}{2}}(\mathrm{Curl}, \partial\Omega)$ and $H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega)$. Recall for smooth vector fields the partial integration formula (2.2.2). If V is a gradient field, i.e. $V = \nabla u$ for some smooth function u, we arrive with $\mathrm{curl}\, \nabla u = 0$ at

$$\int_{\Omega} \mathrm{curl}\, E \cdot \nabla u \,\mathrm{d}x = \int_{\partial\Omega} (\nu \times E) \cdot \mathrm{Grad}_{\partial\Omega}\, u \,\mathrm{d}s = -\int_{\partial\Omega} \mathrm{Div}_{\partial\Omega}(\nu \times E) u \,\mathrm{d}s.$$

Again, the left hand side does make sense in $H(\mathrm{curl}, \Omega)$, therefore the right trace space has to include the fact, that the trace $\gamma_t E$ admits surface divergence. For smooth vector fields E, we have

$$\nu \times \gamma_T E = \gamma_t E \quad \text{on } \partial\Omega.$$

Therefore, $\gamma_T E$ has to possess the surface rotation $\mathrm{Curl}_{\partial\Omega}$ in the right trace space. Recall the definition of $H^s(\mathrm{Div}, K)$ with $K = (-\pi, \pi)^2$ for the localized tangential vector fields as the completion of the trigonometric vector polynomials $\mathcal{T}(K, \mathbb{C}^2)$. K can be seen as surface of the three-dimensional cube $(-\pi, \pi)^3$. If we consider the trigonometric vector monomial

$$F(x) = f\mathrm{e}^{\mathrm{i}n\cdot x}, \quad x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \in K, \quad f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \in \mathbb{C}^2, \quad n = \begin{pmatrix} n_1 \\ n_2 \end{pmatrix} \in \mathbb{Z}^2$$

we can easily extend F to a vector field defined on $(-\pi, \pi)^3$ by forgetting the third variable and setting the third component to zero, i.e.

$$F(y) = (F(\hat{y}), 0)^\top \in \mathbb{C}^3, \quad y \in (-\pi, \pi)^3 \subset \mathbb{R}^3,$$

where $\hat{y} = (y_1, y_2)^\top \in K$. The surface divergence $\mathrm{Div}_K F$ is then given by

$$\mathrm{Div}_K F(x) = \mathrm{i}(n \cdot f)\mathrm{e}^{\mathrm{i}n\cdot x}.$$

This motivates the second term in the $H^s(\mathrm{Div}, K)$-norm. For the surface rotation $\mathrm{Curl}_K F$, we have analogously

$$\mathrm{Curl}_K F(x) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 0 \\ \mathrm{i}(n_1 f_2 - n_2 f_1) \end{pmatrix} \mathrm{e}^{\mathrm{i}n\cdot x} = \mathrm{i}(n \times f)\mathrm{e}^{\mathrm{i}n\cdot x},$$

which motivates the second term in the $H^s(\mathrm{Curl}, K)$-norm. The boundedness of the surface divergence and the surface rotation is the reason, why these operators can be extended to linear bounded operators between certain Sobolev spaces on the boundary $\partial\Omega$ for Lipschitz domains. Since the above definitions used boundaries of class C^2, we have to redefine the surface differential operators in the context of Lipschitz domains. We will summarize this in the following theorem.

Theorem 2.6 (Surface differential operators)**.** *Let Ω be a bounded Lipschitz domain with boundary $\partial\Omega$. Let $\psi \in H^1(\Omega)$. Then $\nabla\psi \in H(\mathrm{curl}, \Omega)$. We define the bounded linear operators* $\mathrm{Grad}_{\partial\Omega}$ *and* $\overrightarrow{\mathrm{Curl}}_{\partial\Omega}$ *by*

$$\mathrm{Grad}_{\partial\Omega} : H^{\frac{1}{2}}(\partial\Omega) \to H^{-\frac{1}{2}}(\mathrm{Curl}, \partial\Omega)$$

$$\overrightarrow{\mathrm{Curl}}_{\partial\Omega} : H^{\frac{1}{2}}(\partial\Omega) \to H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega)$$

by

$$\mathrm{Grad}_{\partial\Omega}\,\varphi = \gamma_T \nabla\eta\varphi \quad \text{and} \quad \overrightarrow{\mathrm{Curl}}_{\partial\Omega}\varphi = \gamma_t \nabla\eta\varphi.$$

We define the linear bounded functionals

$$\mathrm{Div}_{\partial\Omega} : H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega) \to H^{-\frac{1}{2}}(\partial\Omega), \quad \mathrm{Curl}_{\partial\Omega} : H^{-\frac{1}{2}}(\mathrm{Curl}, \partial\Omega) \to H^{-\frac{1}{2}}(\partial\Omega)$$

by

$$_{H^{-\frac{1}{2}}(\partial\Omega)}\langle \mathrm{Div}_{\partial\Omega}\,\varphi, \psi\rangle_{H^{\frac{1}{2}}(\partial\Omega)} = {}_{H^{-\frac{1}{2}}(\mathrm{Div},\partial\Omega)}\langle -\varphi, \mathrm{Grad}_{\partial\Omega}\,\psi\rangle_{H^{-\frac{1}{2}}(\mathrm{Curl},\partial\Omega)}$$

and

$$_{H^{-\frac{1}{2}}(\partial\Omega)}\langle \mathrm{Curl}_{\partial\Omega}\,\varphi, \psi\rangle_{H^{\frac{1}{2}}(\partial\Omega)} = {}_{H^{-\frac{1}{2}}(\mathrm{Div},\partial\Omega)}\langle \overrightarrow{\mathrm{Curl}}_{\partial\Omega}\psi, -\varphi\rangle_{H^{-\frac{1}{2}}(\mathrm{Curl},\partial\Omega)}$$

for all $\psi \in H^{\frac{1}{2}}(\partial\Omega)$.

Proof. Since $\mathrm{curl}\,\nabla\varphi = 0$ in $L^2(\Omega)$ for $\varphi \in H^1(\Omega)$, see [39, Theorem 3.40], we have $\nabla\eta\varphi \in H(\mathrm{curl}, \Omega)$. The boundedness of $\mathrm{Grad}_{\partial\Omega}$ and $\overrightarrow{\mathrm{Curl}}_{\partial\Omega}$ follows from the boundedness of $\eta : H^{\frac{1}{2}}(\partial\Omega) \to H^1(\Omega)$. The boundedness of $\mathrm{Div}_{\partial\Omega}$ and $\mathrm{Curl}_{\partial\Omega}$ follows immediately. If φ can be extended to a smooth function in the neighborhood of $\partial\Omega$, then $\mathrm{Grad}_{\partial\Omega}$, defined as in this theorem, is just the classic surface gradient, which does not depend on the extension, see [33, Lemma A.19]. By a density argument we conclude that the definition of the surface differential operators in this theorem does not depend on the choice of η. □

2.3. Analytic solutions and the Calderón operator

The scattering problems defined in Section 2.1 are formulated in unbounded domains in $\mathbb{R}^3$. In this section, a summary of [39, Section 9.3], we want to present the framework, which allows us to consider weak formulations of those scattering problems in bounded domains in $\mathbb{R}^3$. This is possible, since we can find explicit representations of solutions of Maxwell's equations in linear isotropic homogeneous media, such as vacuum. Recall, that we always assumed our scatterer to be surrounded by such a medium. In this section, let $R > 0$ be large enough, that the scatterer D lies completely in the ball of radius R centered in 0, i.e. $\overline{D} \subset B_R(0)$. We are considering the following scattering problem

$$\mathrm{curl}\,E^s - \mathrm{i}k\,H^s = 0 \quad \text{in } \mathbb{R}^3 \setminus \overline{B_R(0)}, \tag{2.3.1a}$$

$$\operatorname{curl} H^s + \mathrm{i}k\, E^s = 0 \quad \text{in } \mathbb{R}^3 \setminus \overline{B_R(0)}, \tag{2.3.1b}$$

$$\nu \times E^s = g \quad \text{on } \partial B_R(0), \tag{2.3.1c}$$

$$(E^s, H^s) \text{ satisfies SMRC}, \tag{2.3.1d}$$

for a tangential vector field g. For now, we will assume g to be smooth. Later on, we want to choose $g = \nu \times \hat{E}^s$, where $\hat{E}^s$ is the solution of the scattering problem restricted to $B_R(0)$. As we have seen before, see Lemma 2.1, the Maxwell system is closely connected to the Helmholtz equation. In order to find explicit solutions of (2.3.1a)-(2.3.1d), we start by finding solutions of the Helmholtz equation

$$\Delta u + k^2 u = 0, \tag{2.3.2}$$

using *spherical coordinates* (r, θ, φ) defined by

$$\mathbb{R}^3 \ni x = \begin{pmatrix} r \sin\theta \cos\varphi \\ r \sin\theta \sin\varphi \\ r\cos\theta \end{pmatrix}, \quad r > 0,\ \theta \in [0, \pi],\ \varphi \in [0, 2\pi].$$

Since we want to exploit the structure of the spherical coordinates, we make an Ansatz by separation of variables, i.e. $u(x) = u(r, \theta, \varphi) = u_1(r) u_2(\theta, \varphi)$. Then (2.3.2) reads as

$$\frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2 \frac{\partial u_1}{\partial r}\right) + k^2 r^2 u_1\right] u_2 + \left[\frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial u_2}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2 u_2}{\partial \varphi^2}\right] u_1 = 0, \tag{2.3.3}$$

or, using the representation of the Laplace-Beltrami operator in spherical coordinates

$$\frac{1}{u_1}\left[\frac{\partial}{\partial r}\left(r^2 \frac{\partial u_1}{\partial r}\right) + k^2 r^2 u_1\right] + \frac{1}{u_2} \Delta_{\partial B_1(0)} u_2 = 0. \tag{2.3.4}$$

Noticing, that the first summand is a function of only r and the second one of only θ and φ, the sum can only be zero, if there is a constant $\eta \in \mathbb{C}$ such that

$$\Delta_{\partial B_1(0)} u_2 = \eta u_2 \tag{2.3.5a}$$

$$\frac{\partial}{\partial r}\left(r^2 \frac{\partial u_1}{\partial r}\right) + (k^2 r^2 + \eta) u_1 = 0 \tag{2.3.5b}$$

Note that (2.3.5b) is an ordinary differential equation for $r > 0$ and (2.3.5a) is the eigenvalue problem for the Laplace-Beltrami operator. For an arbitrary $\eta \in \mathbb{C}$, this is not solvable. We present the solutions of (2.3.5a) in the following theorem. For completeness, we define the *Legendre polynomials* P_n of order $n \in \mathbb{N}_0$ by

$$P_n(t) = \frac{(-1)^n}{2^n n!} \frac{\mathrm{d}^n}{\mathrm{d}t^n}(1 - t^2)^n, \quad t \in [-1, 1]$$

and the mth *associated Legendre functions* of order n by

$$P_n^m(t) = (1-t^2)^{\frac{m}{2}} \left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^m P_n(t), \quad m = 0, 1, 2, \dots, n, \; t \in [-1, 1].$$

Furthermore, we define the *spherical harmonics* Y_n^m by

$$Y_n^m(\theta, \varphi) = \sqrt{\frac{2n+1}{4\pi} \frac{(n-|m|)!}{(n+|m|)!}} P_n^{|m|}(\cos\theta) \mathrm{e}^{\mathrm{i}m\varphi}$$

for $n \in \mathbb{N}_0$ and $m \in \mathbb{Z}$ with $|m| \leqslant n$. We have the following theorem.

Theorem 2.7 (Eigenvalues of $\Delta_{\partial B_1(0)}$). *For any $n \in \mathbb{N}_0$ and $m \in \mathbb{Z}$ with $|m| \leqslant n$ we have*

$$\Delta_{\partial B_1(0)} Y_n^m = -n(n+1) Y_n^m,$$

i.e. the spherical harmonics of order n are the eigenfunctions of the Laplace-Beltrami operator with respect to the eigenvalue $-n(n+1)$. The set

$$\{Y_n^m : n \in \mathbb{N}_0, \, m \in \mathbb{Z}, \, |m| \leqslant n\}$$

is a complete orthonormal system in $L^2(\partial B_1(0))$.

Proof. See for example Section 2.4.1 in [40]. □

Due to this result, we only have to find solutions of (2.3.5b) for $\eta = -n(n+1)$, $n \in \mathbb{N}_0$. Using the change of variables $t = kr$, one finds two families of solutions, the *spherical Bessel functions* of order $n \in \mathbb{N}_0$, given by

$$j_n(t) = \sum_{l=0}^{\infty} \frac{(-1)^l}{2^l l!} \frac{t^{n+2l}}{(-2n+1)(-2n+3)\cdots(-2n+2l-1)}, \qquad t \in \mathbb{R},$$

and the *spherical Neumann function* of order $n \in \mathbb{N}_0$, given by

$$y_n(t) = -\frac{(2n)!}{2^n n!} \sum_{l=0}^{\infty} \frac{(-1)^l}{2^l l!} \frac{t^{2l-n-1}}{(-2n+1)(-2n+3)\cdots(-2n+2l-1)}$$

for $t > 0$. Note the singularity of the Neumann functions for $t \to 0$. The linear combination

$$h_n^{(1)} = j_n + \mathrm{i} y_n, \quad h_n^{(2)} = j_n - \mathrm{i} y_n, \quad n \in \mathbb{N}_0$$

are called *spherical Hankel functions* of order $n \in \mathbb{N}_0$ of the first and second kind. These functions and their derivatives have the following asymptotic behaviour

$$\begin{aligned} h_n^{(1,2)}(t) &= \frac{1}{t}\mathrm{e}^{\pm\mathrm{i}(t-\frac{n\pi}{2}-\frac{\pi}{2})} + \mathcal{O}\Big(\frac{1}{t^2}\Big), \\ \big(h_n^{(1,2)}\big)'(t) &= \frac{1}{t}\mathrm{e}^{\pm\mathrm{i}(t-\frac{n\pi}{2})} + \mathcal{O}\Big(\frac{1}{t^2}\Big), \end{aligned} \tag{2.3.6}$$

where the positive sign corresponds to the spherical Hankel function of the first kind, and the minus sign to the spherical Hankel function of the second kind, see [14, Section 2.4]. We conclude, that we have constructed to families of functions, namely

$$u_n^m(x) = j_n(kr)Y_n^m(\theta,\varphi), \quad v_n^m(x) = h_n^{(1)}(kr)Y_n^m(\theta,\varphi), \quad n \in \mathbb{N}_0,\ |m| \leqslant n,$$

where the u_n^m satisfy the Helmholtz equation in $\mathbb{R}^3$ and the v_n^m in $\mathbb{R}^3 \setminus \{0\}$. Using the asymptotic behaviour of the v_n^m, one can show the following lemma.

Lemma 2.8. *For $n \in \mathbb{N}_0$ and $m \in \mathbb{Z}$ with $|m| \leqslant n$, we have that v_n^m satisfies the Sommerfeld radiation condition (2.1.3).*

Proof. This follows from the asymptotic behaviour of the Hankel functions (2.3.6), for more details see [14, Theorem 2.9]. □

Recall our goal to construct explicit solution of the scattering problem (2.3.1a)-(2.3.1d). Using our set of solutions of the Helmholtz equation, we arrive at the family of *vector wave functions*, defined in spherical coordinates by

$$\begin{aligned} M_n^m(x) &= \frac{1}{\sqrt{n(n+1)}}\operatorname{curl}(x\, j_n(kr)\, Y_n^m(\theta,\varphi)), \quad x \in \mathbb{R}^3, \\ N_n^m(x) &= \frac{1}{\sqrt{n(n+1)}}\operatorname{curl}(x\, h_n^{(1)}(kr)\, Y_n^m(\theta,\varphi)), \quad x \in \mathbb{R}^3 \setminus \{0\}. \end{aligned}$$

These are called *Debye potentials* and define solutions of the system (2.1.1) in $\mathbb{R}^3$ and $\mathbb{R}^3 \setminus \{0\}$, resp. by the following lemma.

Lemma 2.9. *Let u be a solution of the Helmholtz equation*

$$\Delta u + k^2 u = 0$$

Then $E(x) = \operatorname{curl}(x\, u(x))$ is a solution of

$$\operatorname{curl}^2 E - k^2 E = 0.$$

Proof. Let u be a solution of the Helmholtz equation, i the identity, i.e. $i(x) = x$ and $E(x) = \operatorname{curl}\big(u(x)i(x)\big)$. Using the vector calculus identity

$$\operatorname{curl}(F \times G) = F \operatorname{div}(G) - G \operatorname{div}(F) + J_F G - J_G F$$

for some sufficiently smooth vector fields F, G, we have

$$\begin{aligned}
\operatorname{curl}^2 E &= \operatorname{curl}^3(u\, i) = \operatorname{curl}^2(\nabla u \times i) \\
&= \operatorname{curl}\big(3\nabla u - \Delta u\, i + J_{\nabla u} i - J_i \nabla u\big) \\
&= k^2 \operatorname{curl}(u\, i) + \operatorname{curl}(J_{\nabla u} i).
\end{aligned}$$

Since

$$\begin{aligned}
J_{\nabla u} i &= (J_{\nabla u} - J_{\nabla u}^\top) i + (J_{\nabla u}^\top i + J_i^\top \nabla u) - J_i^\top \nabla u \\
&= \operatorname{curl}(\nabla u) \times i + \nabla(\nabla u^\top i) - \nabla u,
\end{aligned}$$

we conclude

$$\operatorname{curl}^2 E - k^2 E = 0.$$

□

Inspired by the observation

$$\operatorname{curl}(x\, u(x)) = \nabla u \times x,$$

one can see, that the vector wave functions M_n^m and N_n^m can be interpreted as tangential vector fields on $B_1(0)$. Since we have

$$\begin{aligned}
\delta_n^r \delta_m^s = \int_{\partial B_1(0)} Y_n^m \overline{Y_r^s}\, \mathrm{d}s &= -n(n+1) \int_{\partial B_1(0)} \Delta_{\partial B_1(0)} Y_n^m \overline{Y_r^s}\, \mathrm{d}s \\
&= n(n+1) \int_{\partial B_1(0)} \operatorname{Grad}_{\partial B_1(0)} Y_n^m \cdot \overline{\operatorname{Grad}_{\partial B_1(0)} Y_r^s}\, \mathrm{d}s,
\end{aligned}$$

we find that the *spherical surface harmonics* U_n^m, V_n^m, defined for $\hat{x} \in \mathbb{S}^2$ by

$$\begin{aligned}
U_n^m(\hat{x}) &= \frac{1}{\sqrt{n(n+1)}} \operatorname{Grad}_{\partial B_1(0)} Y_n^m(\hat{x}) \\
V_n^m(\hat{x}) &= \hat{x} \times U_n^m(\hat{x})
\end{aligned}$$

form an orthonormal system in the space of tangential vector fields, which we denote by $L_t^2(\partial B_1(0))$. One can also show completeness.

Lemma 2.10. *The set of spherical surface harmonics*

$$\{U_n^m, V_n^m, n \in \mathbb{N}, m \in \mathbb{Z}, |m| \leqslant n\}$$

is a complete orthonormal system in $L_t^2(\partial B_1(0))$.

Proof. See for example [14, Theorem 6.23]. □

The main difference between the vector wave functions M_n^m and N_n^m (and their curls) is the asymptotic behaviour, as stated in the following lemma.

Lemma 2.11. *The functions* N_n^m, $\frac{1}{\mathrm{i}k} \operatorname{curl} N_n^m$ *are radiating solution of the Maxwell system in* $\mathbb{R}^3 \setminus \{0\}$.

Proof. See [14, Theorem 6.24]. □

Now, we have all the ingredients to state the main theorem of this section. Recall, that our main goal was to find explicit representations of a radiating solution of Maxwell's equations outside some ball of radius R, see (2.3.1a)-(2.3.1d).

Theorem 2.12. *Let* E^s *be a solution of (2.3.1a)-(2.3.1d). Then* E^s *has the representation*

$$E^s(x) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \Big(a_n^m N_n^m(x) + b_n^m \frac{1}{\mathrm{i}k} \operatorname{curl} N_n^m(x) \Big), \qquad |x| > R.$$

The series converges uniformly on compact subsets. For the magnetic field, we have

$$H^s(x) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \Big(a_n^m \frac{1}{\mathrm{i}k} \operatorname{curl} N_n^m(x) - b_n^m N_n^m(x) \Big), \qquad |x| > R.$$

Conversely, if the tangential component of this series converge in L^2 *on the sphere of radius* R, *then the series itself converges uniformly on compact subsets of* $|x| > R$. *In this case, the series represent a radiating solution to the Maxwell system.*

Proof. See [14, Theorem 6.25]. □

If we consider the corresponding interior problem

$$\operatorname{curl}^2 E - k^2 E = 0 \quad \text{in } B_R(0), \tag{2.3.7a}$$

$$\nu \times E = g \quad \text{on } \partial B_R(0), \tag{2.3.7b}$$

we have analogous representation as in the theorem above

$$E(x) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \Big(a_n^m M_n^m(x) + b_n^m \frac{1}{\mathrm{i}k} \operatorname{curl} M_n^m(x) \Big), \quad |x| < R,$$
$$H(x) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \Big(a_n^m M_n^m(x) + b_n^m \frac{1}{\mathrm{i}k} \operatorname{curl} M_n^m(x) \Big), \quad |x| < R.$$

These representations allow us, to calculate explicit representations of our scattering problems from Section 2.1, if we restrict ourselves to the special case $D = B_R(0)$. These formulas, which will be presented in Section 2.3.1, are immensely important as a first step of the verification of our numerical experiments.

For now, we will continue presenting the framework for the Calderón operator. In Section 2.2.2, we defined the Sobolev space $H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega)$ for the boundary of a bounded Lipschitz domain. For the special case, where Ω is a ball of some radius, i.e. $\Omega = B_R(0)$, one can give a more direct definition, using the orthonormal systems in $L^2(\partial B_R(0))$ and $L^2_t(\partial B_R(0))$. First, any given $U \in L^2_t(\partial B_R(0))$ can be written by Lemma 2.10 as

$$U(x) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \Big(a_n^m U_n^m(\hat{x}) + b_n^m V_n^m(\hat{x}) \Big), \quad x \in B_R(0),\ \hat{x} = \frac{x}{|x|} \in \mathbb{S}^2$$

with coefficients $a_n^m, b_n^m \in \mathbb{C}$, $n \in \mathbb{N}$, $|m| \leqslant n$. Since the U_n^m and V_n^m are orthonormal, we have

$$\|U\|^2_{L^2_t(\partial B_R(0))} = R^4 \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \Big(|a_n^m|^2 + |b_n^m|^2 \Big).$$

We can calculate the surface divergence of U_n^m by

$$\begin{aligned} \mathrm{Div}_{\partial B_1(0)} U_n^m &= \frac{1}{\sqrt{n(n+1)}} \mathrm{Div}_{\partial B_1(0)} \mathrm{Grad}_{\partial B_1(0)} Y_n^m \\ &= \frac{1}{\sqrt{n(n+1)}} \Delta_{\partial B_1(0)} Y_n^m = -\sqrt{n(n+1)} Y_n^m. \end{aligned}$$

We have $\mathrm{Div}_{\partial B_1(0)} V_n^m = 0$ by considering for $n, k \in N$ and $m, l \in \mathbb{Z}$ with $|m| \leqslant n$ and $|l| \leqslant k$

$$\int_{\partial B_1(0)} \overline{Y_k^l} \, \mathrm{Div}_{\partial B_1(0)} V_n^m \, \mathrm{d}s = - \int_{\partial B_1(0)} V_n^m \cdot \mathrm{Grad}_{\partial B_1(0)} \overline{Y_k^l} \, \mathrm{d}s$$

$$= -\int_{\partial B_1(0)} V_n^m \cdot \overline{U_k^l} \, \mathrm{d}s = 0.$$

We can define $H^s(\mathrm{Div}, \partial B_R(0))$ for $s \in \mathbb{R}$ as the completion of the space of tangential vector fields of the form

$$U = \sum_n \sum_{m=-n}^{n} \left(a_n^m U_n^m + b_n^m V_n^m \right),$$

where the sum over n is finite with respect to the norm

$$\|U\|^2_{H^s(\mathrm{Div}, \partial B_R(0))} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[(n(n+1))^{s+1} |a_n^m|^2 + (n(n+1))^s |b_n^m|^2 \right].$$

Consider for $g \in H^{-\frac{1}{2}}(\mathrm{Div}, \partial B_R(0))$, given by

$$g = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left(\alpha_n^m U_n^m + \beta_n^m V_n^m \right) \tag{2.3.8}$$

the exterior spherical scattering problem (2.3.1a) - (2.3.1d) for some coefficients $\alpha_n^m, \beta_n^m \in \mathbb{C}$, $n \in \mathbb{N}$, $|m| \leqslant n$. By Theorem 2.12, we make the Ansatz

$$\begin{pmatrix} E^s \\ H^s \end{pmatrix}(x) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[a_n^m \begin{pmatrix} N_n^m \\ \frac{1}{\mathrm{i}k} \operatorname{curl} N_n^m \end{pmatrix}(x) + b_n^m \begin{pmatrix} \frac{1}{\mathrm{i}k} \operatorname{curl} N_n^m \\ -N_n^m \end{pmatrix}(x) \right]. \tag{2.3.9}$$

In order to match the boundary condition $\nu \times E^s = g$, we have to calculate the traces $\nu \times N_n^m$ and $\nu \times \frac{1}{\mathrm{i}k} \operatorname{curl} N_n^m$ explicitly. This is done by using the representation of curl in spherical coordinates. We omit the calculation and present the result. We have

$$N_n^m(x) = -h_n^{(1)}(kR) V_n^m(\hat{x})$$

and

$$\frac{1}{\mathrm{i}k} \operatorname{curl} N_n^m(x)$$
$$= \frac{\sqrt{n(n+1)}}{\mathrm{i}kR} h_n^{(1)}(kR) Y_n^m(\hat{x}) \hat{x} + \frac{1}{\mathrm{i}kR} (h_n^{(1)}(kR) + k|x| (h_n^{(1)})'(kR)) U_n^m,$$

for $x = R\hat{x}$, $R > 0$, $\hat{x} \in \mathbb{S}^2$, see [14, Section 6.5]. Therefore, the boundary values are given by

$$\nu \times N_n^m(x) = h_n^{(1)}(kR) U_n^m(\hat{x}),$$

$$\nu \times \frac{1}{\mathrm{i}k} \operatorname{curl} N_n^m(x) = \frac{1}{\mathrm{i}kR}\big(h_n^{(1)}(kR) + kR(h_n^{(1)})'(kR)\big)V_n^m.$$

for $x = R\hat{x}$, $\hat{x} \in \mathbb{S}^2$. If we compare the coefficients in

$$\begin{aligned} 0 = \nu \times E^s - g = &\sum_{n=1}^{\infty} \sum_{m=-n}^{n} (a_n^m h_n^{(1)}(kR) - \alpha_n^m)U_n^m \\ &+ \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \Big(\frac{b_n^m}{\mathrm{i}kR}(h_n^{(1)}(kR) + kR(h_n^{(1)})'(kR)) - \beta_n^m\Big)V_n^m \end{aligned}$$

we find, that the coefficients a_n^m and b_n^m of the solution are formally given by

$$a_n^m = \frac{\alpha_n^m}{h_n^{(1)}(kR)}, \qquad b_n^m = \frac{\mathrm{i}kR\beta_n^m}{h_n^{(1)}(kR) + kR(h_n^{(1)})'(kR)}. \tag{2.3.10}$$

We conclude this with the following lemma.

Lemma 2.13. *Let $k \in \mathbb{R}$. For any $g \in H^{-\frac{1}{2}}(\mathrm{Div}, \partial B_R(0))$ with the representation (2.3.8), the unique solution E^s, H^s of (2.3.1a) - (2.3.1d) is given by (2.3.9) with the coefficients defined in (2.3.10).*

Proof. By Theorem 2.12, we only have to check if the coefficients a_n^m, b_n^m are well defined. Assume $h_n^{(1)}(kR) = 0$ for some $n \in \mathbb{N}$. Since $k, R > 0$, we have by $h_n^{(1)} = j_n + iy_n$ that $j_n(kR) = y_n(kR) = 0$. This is a contradiction to the Wronskian

$$j_n(z)y_n'(z) - j_n'(z)y_n(z) = \frac{1}{z^2}, \quad z \in \mathbb{C}. \tag{2.3.11}$$

Therefore a_n^m is well defined. Analogously, if $h_n^{(1)}(kR) + kR(h_n^{(1)})'(kR) = 0$, we have $j_n(kR) + kRj_n'(kR) = 0$ and $y_n + kRy_n'(kR) = 0$. This leads to

$$-kRy_n'(kR)j_n(kR) = -kRj_n'(kR)y_n(kR).$$

Again by the Wronskian, we conclude

$$0 = kR(y_n'(kR)j_n(kR) - y_n(kR)j_n'(kR)) = \frac{1}{kR},$$

a contradiction. $\square$

We now define the *Calderón operator* Λ as follows. Given a function λ in $H^{-\frac{1}{2}}(\mathrm{Div}, \partial B_R(0))$, we define $\Lambda\lambda = \hat{x} \times H^s$, where the pair (E^s, H^s) satisfies

(2.3.1a) - (2.3.1d) with $g = \lambda$. Due to our representations, we can define $\Lambda\lambda$ in terms of the coefficients α_n^m, β_n^m in the representation

$$\lambda = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left(\alpha_n^m U_n^m + \beta_n^m V_n^m\right)$$

by

$$\begin{aligned}\Lambda\lambda = \hat{x} \times H^s = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \Bigg[& \frac{\alpha_n^m}{\mathrm{i}kR} \frac{h_n^{(1)}(kR) + kR(h_n^{(1)})'(kR)}{h_n^{(1)}(kR)} V_n^m \\ & - \mathrm{i}kR\, \beta_n^m \frac{h_n^{(1)}(kR)}{h_n^{(1)}(kR) + kR(h_n^{(1)})'(kR)} U_n^m \Bigg].\end{aligned}$$

The next theorem is a summary of the properties of Λ.

Theorem 2.14. *The Calderón Operator*

$$\Lambda : H^{-\frac{1}{2}}(\mathrm{Div}, \partial B_R(0)) \mapsto H^{-\frac{1}{2}}(\mathrm{Div}, \partial B_R(0))$$

is linear and bounded.

Proof. See [39, Theorem 9.21]. □

The Calderón operator will help us in Section 2.4 to incorporate the Silver-Müller radiation condition into the weak formulation. For now, we continue to present analytic solutions to scattering problems, since that requires the same Ansatz and the comparison of coefficients, as we have done to define the Calderón operator.

2.3.1. Analytic solutions

Throughout this section, we consider positive wavenumbers $k > 0$ and the scatterer $D = B_R(0)$ for some $R > 0$. Furthermore, we will always use the decomposition

$$\begin{pmatrix} E^i \\ H^i \end{pmatrix}(x) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[\alpha_n^m \begin{pmatrix} M_n^m \\ \frac{1}{\mathrm{i}k} \operatorname{curl} M_n^m \end{pmatrix}(x) + \beta_n^m \begin{pmatrix} \frac{1}{\mathrm{i}k} \operatorname{curl} M_n^m \\ -M_n^m \end{pmatrix}(x) \right] \tag{2.3.12}$$

of the incoming field in a neighborhood of ∂D, which holds on any compact set. We already stated the solution to the spherical perfect conductor in Lemma 2.13 and continue with the impedance boundary condition.

Lemma 2.15. *Let $k, \lambda \in \mathbb{R}$. For any pair of incoming fields with representation (2.3.12), the unique solution of (2.1.6a) - (2.1.6c) is given by*

$$\begin{pmatrix} E^s \\ H^s \end{pmatrix}(x) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[a_n^m \begin{pmatrix} N_n^m \\ \frac{1}{\mathrm{i}k} \operatorname{curl} N_n^m \end{pmatrix}(x) + b_n^m \begin{pmatrix} \frac{1}{\mathrm{i}k} \operatorname{curl} N_n^m \\ -N_n^m \end{pmatrix}(x) \right],$$

where the coefficients a_n^m, $b_n^m \in \mathbb{C}$ are given by

$$a_n^m = -\alpha_n^m \frac{j_n(kR) + kR\, j_n'(kR) + \mathrm{i}\lambda kR j_n(kR)}{h_n^{(1)}(kR) + kR\,(h_n^{(1)})'(kR) + \mathrm{i}\lambda kR h_n^{(1)}(kR)}$$

$$b_n^m = -\beta_n^m \frac{\lambda\big(j_n(kR) + kR\, j_n'(kR)\big) + \mathrm{i}kR\, j_n(kR)}{\lambda\big(h_n^{(1)}(kR) + kR\,(h_n^{(1)})'(kR)\big) + \mathrm{i}kR\, h_n^{(1)}(kR)}$$

for $n \in \mathbb{N}$, $|m| \leqslant n$.

Proof. If we plug in the Ansatz for the incoming and scattered field into the boundary condition

$$\nu \times (H^s + H^i) = \lambda \nu \times \big((E^s + E^i) \times \nu\big)$$

and use $\nu \times (U \times \nu) = U$ for tangential vector fields as well as $\nu \times V_n^m = U_n^m$, we can conclude the representations of a_n^m and b_n^m by comparing coefficients. We have to check, whether the denominator in the claimed representations can vanish. Let the denominator of the representation of α_n^m vanish for some $n \in \mathbb{N}$. Then we define the scalar function

$$u_n(x) = R\, h_n^{(1)}(k|x|) Y_n^m\Big(\frac{x}{|x|}\Big), \quad x \neq 0.$$

By Lemma 2.8, we have hat u_n is a radiating solution of

$$\begin{aligned} \Delta u + k^2 u = 0, &\quad \text{in } \mathbb{R}^3 \setminus \overline{B_R(0)}, \\ \frac{\partial u}{\partial \nu} + \widehat{\lambda} u = 0, &\quad \text{on } \partial B_R(0), \end{aligned}$$

with $\hat{\lambda} = \frac{1 + \mathrm{i}k\lambda R}{R}$. We have by [13, Theorem 3.37], that any radiating solution has to vanish, i.e. $u_n \equiv 0$. This is a contradiction. Analogously, defining $u_n = \lambda R\, h_n^{(1)}(k|x|) Y_n^m(x/|x|)$ and considering $\widehat{\lambda} = \frac{\lambda + \mathrm{i}kR}{\lambda R}$, we conclude that also the second denominator can not vanish. ☐

We continue with the scattering from penetrable obstacles. Since we now have additionally a non trivial electric and magnetic field inside of the scatterer, we have to expand our Ansatz. The vector wave functions depend of course on the wavenumber. The scattering from penetrable obstacles involves two wavenumbers, the exterior k and the interior κ. Therefore, we will denote this by $M_n^m(x,k)$ and $M_n^m(x,\kappa)$, respectively. κ is called *interior (Dirichlet) eigenvalue*, if the boundary value problem

$$\begin{aligned} &\operatorname{curl}^2 E - \kappa^2 E = 0, \quad \text{in } B_R(0) \\ &\nu \times E = 0, \quad \text{on } \partial B_R(0) \end{aligned}$$

admits non-trivial solutions. For the next theorem we assume, that κ is no interior eigenvalue.

Lemma 2.16. *Let ε_D, ε_0, μ_D and $\mu_0 \in \mathbb{R}$ and $\sigma_D = 0$. Furthermore, let κ be no interior Dirichlet eigenvalue. For any pair of incoming fields with representation (2.3.12), the unique solution of (2.1.5a) - (2.1.5e) is given by*

$$\begin{pmatrix} E^s \\ H^s \end{pmatrix}(x) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\left[a_n^m \begin{pmatrix} N_n^m \\ \frac{1}{\mathrm{i}k}\operatorname{curl} N_n^m \end{pmatrix}(x,k) + b_n^m \begin{pmatrix} \frac{1}{\mathrm{i}k}\operatorname{curl} N_n^m \\ -N_n^m \end{pmatrix}(x,k)\right]$$

for $x \in \mathbb{R}^3 \setminus \overline{D}$ and by

$$\begin{pmatrix} E \\ H \end{pmatrix}(x) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\left[c_n^m \begin{pmatrix} M_n^m \\ \frac{1}{\mathrm{i}k}\operatorname{curl} M_n^m \end{pmatrix}(x,\kappa) + d_n^m \begin{pmatrix} \frac{1}{\mathrm{i}k}\operatorname{curl} M_n^m \\ -M_n^m \end{pmatrix}(x,\kappa)\right]$$

for $x \in D$, where the coefficients a_n^m, b_n^m, c_n^m, $d_n^m \in \mathbb{C}$ are the unique solutions of the linear systems

$$A_n^m \begin{pmatrix} a_n^m & b_n^m & c_n^m & d_n^m \end{pmatrix}^\top = e_n^m$$

with the matrix $A_n^m \in \mathbb{C}^{4\times 4}$ given by

$$A_n^m = \begin{pmatrix} H_n(kR) & -\sqrt{\frac{\varepsilon_0}{\varepsilon_D}\frac{\mu_0}{\mu_D}}J_n(\kappa R) & 0 & 0 \\ h_n^{(1)}(kR) & -\sqrt{\frac{\varepsilon_0}{\varepsilon_D}}j_n(\kappa R) & 0 & 0 \\ 0 & 0 & H_n(kR) & -\sqrt{\frac{\mu_0}{\mu_D}\frac{\varepsilon_0}{\varepsilon_D}}J_n(\kappa R) \\ 0 & 0 & h_n^{(1)}(kR) & -\sqrt{\frac{\mu_0}{\mu_D}}j_n(\kappa R) \end{pmatrix},$$

where we abbreviated $J_n(z) = j_n(z) + z j_n'(z)$ and $H_n(z) = h_n^{(1)}(z) + z(h_n^{(1)})'(z)$. The right hand side $e_n^m \in \mathbb{C}^4$ is given by

$$e_n^m = -\begin{pmatrix} J_n(kR)\alpha_n^m & -j_n(kR)\alpha_n^m & -J_n(kR)\beta_n^m & -j_n(kR)\beta_n^m \end{pmatrix}^\top.$$

Proof. We plug in our Ansatz into the transmission conditions. This leads by orthogonality of the vector spherical harmonics to the decoupled linear systems stated above. We will now prove that the linear system is always uniquely solvable. The determinant of A_n^m is given by the product of the determinant of the upper left block, given by

$$-\sqrt{\frac{\varepsilon_0}{\varepsilon_D}}\big(H_n(kR)j_n(\kappa R)-\frac{\mu_0}{\mu_D}J_n(\kappa R)h_n^{(1)}(kR)\big) \tag{2.3.13}$$

and the lower right block, given by

$$-\sqrt{\frac{\mu_0}{\mu_D}}\big(H_n(kR)j_n(\kappa R)-\frac{\varepsilon_0}{\varepsilon_D}J_n(\kappa R)h_n^{(1)}(kR)\big). \tag{2.3.14}$$

Assuming $\det A_n^m = 0$, we have that one of the determinants (2.3.13) or (2.3.14) has to be zero. Let (2.3.13) be zero. Since all material parameter are real valued, we can split it into real and imaginary part and arrive at

$$0=\Big(1-\frac{\mu_0}{\mu_D}\Big)j_n(kR)j_n(\kappa R)+kR\,j_n(\kappa R)j_n'(kR)-\frac{\mu_0}{\mu_D}\kappa R\,j_n'(\kappa R)j_n(kR), \tag{2.3.15}$$

$$0=\Big(1-\frac{\mu_0}{\mu_D}\Big)y_n(kR)j_n(\kappa R)+kR\,j_n(\kappa R)y_n'(kR)-\frac{\mu_0}{\mu_D}\kappa R\,j_n'(\kappa R)y_n(kR). \tag{2.3.16}$$

Since κ is no interior eigenvalue, we have $j_n(\kappa R)\neq 0$ for all $n\in\mathbb{N}$, since otherwise $M_n^m(x,\kappa)$ is a non-trivial solution of the interior Dirichlet problem. If $j_n(kR)$ were zero, we could conclude by (2.3.15) that $j_n(\kappa R)$ has to be zero, since $j_n'(kR)$ can not also be zero by the Wronskian. So $j_n(kR)$ can not vanish for any $n\in\mathbb{N}$. Similarly, if $y_n(kR)=0$, we can conclude $y_n'(kR)=0$ by (2.3.16), which also can not be. So we can divide the first equation by the product of $j_n(kR)$ and $j_n(\kappa R)$ and the second one by the product of $y_n(kR)$ and $j_n(\kappa R)$ and subtract them. This yields with the Wronskian (2.3.11)

$$0=kR\big(j_n'(kR)y_n(kR)-j_n(kR)y_n'(kR)\big)=-\frac{1}{kR},$$

a contradiction. Repeating the same argument with (2.3.14), we conclude $\det A_n^m\neq 0$. □

Our Ansatz uses solutions of the Maxwell system (2.0.5) and then matches the boundary conditions. This does not work directly for chiral media. One can transform solutions of the scattering from chiral media (2.1.7a) - (2.1.7e) to solutions of a certain transmission problem, see [5]. This will also be addressed later in Section 5.

2.4. Weak formulations

In this section, we want to present the formulations for the scattering problems. We start with the perfect conductor. As mentioned above, we can consider Lipschitz domains. So let D be a bounded, simply connected Lipschitz domain. Let $R > 0$ be large enough such that $\overline{D} \subset B_R(0)$ and define the open set $\Omega = B_R(0) \setminus \overline{D}$. Note that Ω has the two connected boundaries ∂D and $\partial B_R(0)$.

2.4.1. Perfect conductor

Recall the scattering problem of the perfect conductor (2.1.4a) - (2.1.4c):

$$\operatorname{curl} E = \mathrm{i}k\,H, \quad \operatorname{curl} H = -\mathrm{i}k\,E \quad \text{in } \mathbb{R}^3 \setminus \overline{D}, \tag{2.4.1a}$$

$$\nu \times E = 0 \quad \text{on } \partial D, \tag{2.4.1b}$$

$$\begin{pmatrix} E^s \\ H^s \end{pmatrix} = \begin{pmatrix} E - E^i \\ H - H^i \end{pmatrix} \quad \text{satisfies SMRC.} \tag{2.4.1c}$$

The first equation (2.4.1a) does make sense for E, H in $H(\operatorname{curl}, \Omega)$. The boundary condition (2.4.1b) can be understood as $\gamma_t E = 0$ in $H^{-\frac{1}{2}}(\operatorname{Div}, \partial D)$. Therefore, we choose the closed subspace

$$H_{\mathrm{pc}}(\Omega) := \{E \in H(\operatorname{curl}, \Omega) : \gamma_t E = 0\}. \tag{2.4.2}$$

For now, let (E, H) be a pair of smooth solutions of (2.4.1a) - (2.4.1c) and let V be a smooth vector field with $\nu \times V = 0$ on ∂D. We multiply the second equation of (2.4.1a) with $\overline{V}$ and use the partial integration formula (2.2.2) and arrive at

$$\begin{aligned} 0 &= \int_\Omega (\operatorname{curl} H + \mathrm{i}kE) \cdot \overline{V}\,\mathrm{d}x \\ &= \int_\Omega \left(H \cdot \overline{\operatorname{curl} V} + \mathrm{i}kE \cdot \overline{V}\right) \mathrm{d}x - \int_{\partial D} (\nu \times H) \cdot \overline{V}\,\mathrm{d}s + \int_{\partial B_R(0)} (\nu \times H) \cdot \overline{V}\,\mathrm{d}s. \end{aligned}$$

Note the minus sign in front of the boundary integral over ∂D since the outwards directed normal vector to ∂D is pointing into Ω. The first boundary integral vanishes, since $\nu \times V = 0$. On the second one, we employ the Calderón operator by

$$\begin{aligned} \nu \times H &= \nu \times (H^s + H^i) \\ &= \Lambda(\nu \times E^s) + \nu \times H^i = \Lambda(\nu \times E) + \nu \times H^i - \Lambda(\nu \times E^i). \end{aligned}$$

Furthermore, we use the first equation of (2.4.1a) to remove H from the equation. After multiplying with ik, we arrive finally at

$$\int_\Omega \left(\operatorname{curl} E \cdot \overline{\operatorname{curl} V} - k^2 E \cdot \overline{V}\right) \mathrm{d}x + \mathrm{i}k \int_{\partial B_R(0)} \Lambda(\nu \times E) \cdot \overline{V} \,\mathrm{d}s$$
$$= \int_{\partial B_R(0)} \left(\mathrm{i}k\Lambda(\nu \times E^i) - \nu \times \operatorname{curl} E^i\right) \cdot \overline{V} \,\mathrm{d}s. \quad (2.4.3)$$

Note, that we have removed the magnetic field from the equation and that the equation can be extended to $E, V \in H_{\mathrm{pc}}(\Omega)$. Note that the boundary integrals become the dual pairings between the trace spaces $H^{-\frac{1}{2}}(\mathrm{Div}, \partial B_R(0)\}$ and $H^{-\frac{1}{2}}(\mathrm{Curl}, \partial B_R(0)\}$. We define the bounded sesquilinear form $\mathcal{A} : H_{\mathrm{pc}}(\Omega) \times H_{\mathrm{pc}}(\Omega) \to \mathbb{C}$ and the antilinear map $\ell : H_{\mathrm{pc}}(\Omega) \to \mathbb{C}$ such that (2.4.3) reads as

$$\mathcal{A}(E, V) = \ell(V). \quad (2.4.4)$$

A *weak solution* of the scattering from a perfect conductor is then a function $E \in H_{\mathrm{pc}}(\Omega)$ such that (2.4.3) holds for all $V \in H_{\mathrm{pc}}(\Omega)$. There exists always a unique solution of (2.4.4), see [39, Theorem 10.7].

2.4.2. Obstacle with impedance boundary condition

Recall the scattering problem involving obstacles with impedance boundary condition (2.1.6a) - (2.1.6c):

$$\operatorname{curl} E = \mathrm{i}k\, H, \quad \operatorname{curl} H = -\mathrm{i}k\, E \quad \text{in } \mathbb{R}^3 \setminus \overline{D}, \quad (2.4.5a)$$
$$\nu \times H = \lambda\big(\nu \times (E \times \nu)\big) \quad \text{on } \partial D, \quad (2.4.5b)$$
$$\begin{pmatrix} E^s \\ H^s \end{pmatrix} = \begin{pmatrix} E - E^i \\ H - H^i \end{pmatrix} \quad \text{satisfies SMRC.} \quad (2.4.5c)$$

The boundary condition (2.4.5b) can not be extended for $E, H \in H(\mathrm{curl}, \Omega)$ since the traces γ_t and γ_T have different range spaces, see Theorem 2.5. We have to impose additional regularity of the solutions in order to formulate a weak formulation as opposed to the perfect conductor case. The space

$$H_{\mathrm{imp}}(\Omega) = \{E \in H(\mathrm{curl}, \Omega) : \nu \times E \in L^2_t(\partial D)\}, \quad (2.4.6)$$

equipped with the inner product

$$\langle \cdot, \cdot \rangle_{H_{\mathrm{imp}}(\Omega)} = \langle \cdot, \cdot \rangle_{H(\mathrm{curl},\Omega)} + \langle \nu \times \cdot, \nu \times \cdot \rangle_{L^2(\partial D)}$$

seems reasonable. Again, let (E, H) be a pair of smooth solutions of (2.4.5a) - (2.4.5c) and V be a smooth vector field. Multiplying the Maxwell system with

$\overline{V}$, partial integration formula (2.2.2) and applying the boundary condition (2.4.5b) leads to

$$0 = \int_\Omega \big(H\cdot\overline{\operatorname{curl} V} + \mathrm{i}kE\cdot V\big)\,\mathrm{d}x - \int_{\partial D} \lambda\big(\nu\times(E\times\nu)\big)\cdot\overline{V}\,\mathrm{d}s + \int_{\partial B_R(0)} (\nu\times H)\cdot\overline{V}\,\mathrm{d}s.$$

We apply again the Calderón operator on the outer boundary $\partial B_R(0)$ and remove H from the first volume integral by the first equation of the Maxwell system (2.4.5a). This leads finally to

$$\int_\Omega \big(\operatorname{curl} E\cdot\overline{\operatorname{curl} V} - k^2 E\cdot\overline{V}\big)\,\mathrm{d}x + \mathrm{i}k\int_{\partial B_R(0)} \Lambda(\nu\times E)\cdot\overline{V}\,\mathrm{d}s$$
$$- \mathrm{i}k\int_{\partial D} \lambda(\nu\times E)\cdot(\nu\times\overline{V})\,\mathrm{d}s = \ell(V). \quad (2.4.7)$$

Note that (2.4.7) can be extended to $E, V \in H_{\mathrm{imp}}(\Omega)$. The boundary integral on $\partial B_R(0)$ becomes again the dual pairing between the range spaces of the trace operators γ_t, γ_T. The boundary integral over ∂D is well defined, since $\nu\times E$, $\nu\times V \in L^2_t(\partial D)$. We define the bounded sesquilinear form $\mathcal{B} : H_{\mathrm{imp}}(\Omega)\times H_{\mathrm{imp}}(\Omega) \to \mathbb{C}$ such that (2.4.7) reads as

$$\mathcal{B}(E, V) = \ell(V). \quad (2.4.8)$$

A *weak solution* of the scattering problem from an obstacle with impedance boundary condition is a function $E \in H_{\mathrm{imp}}(\Omega)$ such that (2.4.8) holds for all $V \in H_{\mathrm{imp}}(\Omega)$. There exists always a unique solution of (2.4.8), see [9].

2.4.3. Chiral media

We define the piecewise constant parameters ε_r, μ_r, $\beta_r : \mathbb{R}^3 \setminus \partial D \to \mathbb{C}$ by

$$\varepsilon_r(x) = \begin{cases} \frac{\varepsilon_D}{\varepsilon_0}, & x\in D \\ 1, & x\notin \overline{D} \end{cases}, \qquad \mu_r(x) = \begin{cases} \frac{\mu_D}{\mu_0}, & x\in D \\ 1, & x\notin \overline{D} \end{cases}$$

and

$$\beta_r(x) = \begin{cases} \beta, & x\in D \\ 0, & x\notin \overline{D} \end{cases}.$$

Using the scaling $E = \sqrt{\varepsilon_0}\hat{E}$ and $H = \sqrt{\mu_0}\hat{H}$, the scattering from chiral media (2.1.7a) - (2.1.7e) can be formulated as

$$\begin{cases} \operatorname{curl} E = \mathrm{i}k\mu_r(H + \beta_r \operatorname{curl} H) \\ \operatorname{curl} H = -\mathrm{i}k\varepsilon_r(E + \beta_r \operatorname{curl} E) \end{cases} \quad \text{in } \mathbb{R}^3\setminus\partial D \quad (2.4.9a)$$

$$\nu \times E\big|_+ - \nu \times E\big|_- = 0, \quad \nu \times H\big|_+ - \nu \times H\big|_- = 0 \quad \text{on } \partial D \tag{2.4.9b}$$

$$\begin{pmatrix} E^s \\ H^s \end{pmatrix} = \begin{pmatrix} E - E^i \\ H - H^i \end{pmatrix} \quad \text{satisfies SMRC.} \tag{2.4.9c}$$

As usual, $k = \omega\sqrt{\varepsilon_0 \mu_0}$ denotes the exterior wavenumber. Note that for $\beta = 0$, this scattering problems becomes the scattering from a penetrable obstacle with $\sigma_D = 0$. Considering again smooth solutions (E, H) of (2.4.9a) - (2.4.9c) and a smooth vector field V, we start with the second equation of the Maxwell system (2.4.9a), multiply it by V and use partial integration (2.2.2) in D and Ω. Note, that due to the jumps in the coefficients, we can not expect (E, H) to be smooth in $\mathbb{R}^3$, but only smooth in D and $\mathbb{R}^3 \setminus \overline{D}$. This leads to

$$\begin{aligned} 0 = &\int_{B_R(0)} \Big(H \cdot \overline{\operatorname{curl} V} + \mathrm{i}k\varepsilon_r (E + \beta_r \operatorname{curl} E) \cdot \overline{V} \Big) \, \mathrm{d}x \\ &+ \int_{\partial D} (\nu \times H\big|_+ - \nu \times H\big|_-) \cdot \overline{V} \, \mathrm{d}s + \int_{\partial B_R(0)} \nu \times H \cdot \overline{V} \, \mathrm{d}s. \end{aligned} \tag{2.4.10}$$

The boundary integral on ∂D vanishes due to the transmission condition (2.4.9b). We use a combination of the Maxwell system (2.4.9a) to remove H from the volume integrals and apply the Calderón operator on the boundary. We arrive, after multiplying with $\mathrm{i}k$, at

$$\begin{aligned} &\int_{B_R(0)} \Big[\Big(\frac{1}{\mu_r} - k^2 \beta_r^2 \varepsilon_r \Big) \operatorname{curl} E \cdot \overline{\operatorname{curl} V} - k^2 \varepsilon_r \beta_r \big(E \cdot \overline{\operatorname{curl} V} + \operatorname{curl} E \cdot \overline{V} \big) \Big] \, \mathrm{d}x \\ &\quad - \int_{B_R(0)} k^2 \varepsilon_r E \cdot \overline{V} \, \mathrm{d}x + \mathrm{i}k \int_{\partial B_R(0)} \Lambda(\nu \times E) \cdot \overline{V} \, \mathrm{d}s = \ell(V). \end{aligned} \tag{2.4.11}$$

Note that (2.4.11) can be extended to $E, V \in H(\operatorname{curl}, B_R(0))$. We define the bounded sesquilinear form $\mathcal{C} : H(\operatorname{curl}, B_R(0)) \times H(\operatorname{curl}, B_R(0)) \to \mathbb{C}$ such that (2.4.11) reads as

$$\mathcal{C}(E, V) = \ell(V). \tag{2.4.12}$$

A *weak solution* of the scattering problem for an obstacle consisting of chiral media is a function $E \in H(\operatorname{curl}, B_R(0))$ such that (2.4.12) holds for all $V \in H(\operatorname{curl}, B_R(0))$. Unique solvability of the scattering problem has been shown for C^2 boundaries in [5].

3. Domain Derivatives

This chapter is concerned with the following question: How do the solutions of the scattering problems presented in Section 2.1 behave with respect to variations of the boundary ∂D. We will show that, under certain assumptions on the regularity of the boundary and the regularity of the perturbations of the boundary, we have differentiability of the solutions with respect to the boundary. There have been used several approaches successfully in order to answer this question for acoustic and electromagnetic scattering. One is based on boundary integral equations and investigations on the behaviour of the potentials. For acoustic scattering, see [43, 45]. For electromagnetic scattering, we refer to [44, 16]. Another approach, based on representation formulas, is presented for the acoustic case in [36] and was later applied to electromagnetic cases in [34, 20, 10]. A unified approach for acoustic and electromagnetic scattering using techniques from differential geometry was recently presented in [30]. Our approach, based on variational formulations, was first used for the acoustic scattering from an obstacle with Dirichlet boundary conditions in [32] and later extended and generalized in [25]. This approach as also been successfully used to characterize the shape derivative for the scattering from a penetrable obstacle in the electromagnetic case, see [26]. In this section, we apply and extend the techniques used in [26] to the scattering problems from Section 2.1. For the perfect conductor, we also prove the existence and give a characterization of the second derivative, following again the methods used for acoustic scattering in [25, 27].

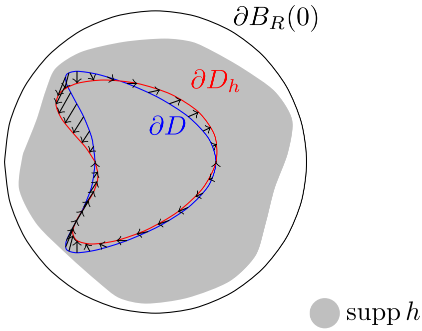

Figure 3.1: Kite D perturbed by h.

Before we start, we present some notations used throughout this section. Let h denote a small C^1 vector field, compactly supported in a neighborhood of ∂D. We will use this vector field as a perturbation of the scatterer D. Given a set $M \subset \mathbb{R}^3$, we denote by M_h the corresponding set perturbed by h, i.e.

$$M_h = \{x + h(x) : x \in M\}.$$

We will always assume $\|h\|_{C^1(\mathbb{R}^3,\mathbb{R}^3)}$ to be small such that the transformation

$$x \mapsto \varphi(x) = x + h(x)$$

is a diffeomorphism. We will consider solutions of the scattering problems with respect to the scatterer D and D_h and investigate their behavior for $\|h\|_{C^1(\mathbb{R}^3,\mathbb{R}^3)} \to 0$. We will use the shortened notation $\|h\|_{C^1}$ for the norm $\|h\|_{C^1(\mathbb{R}^3,\mathbb{R}^3)}$. Recall the weak formulations for the scattering problems defined in a bounded domain, where the outer boundary is the surface of $B_R(0)$ for some $R > 0$, see Section 2.4. Throughout this section, we will always assume, that the compact support of h is in $B_R(0)$, i.e $h \equiv 0$ in a neighborhood of $\partial B_R(0)$. This is always possible by choosing R large enough. See Figure 3.1 for an example.

Considering M and M_h related by the transformation φ, we define for a function $f : M_h \to \mathbb{R}^d$ with $d \in \mathbb{N}$ the function $\widetilde{f} : M \to \mathbb{R}^d$ by

$$\widetilde{f}(x) = \big(f \circ \varphi\big)(x) = f(\varphi(x)) = f(x + h(x)).$$

We can decompose a continuous vector field $F : \partial D \to \mathbb{C}^3$ into normal and tangential components by

$$F = F_\tau + F_\nu \nu = \nu \times (F \times \nu) + (F \cdot \nu)\nu.$$

Note, that formally $\gamma_T F = F_\tau$ holds, but the left hand side might be an element of $H^{-\frac{1}{2}}(\mathrm{Curl}, \partial D)$. We will use the notation F_τ for a tangential vector field in $L^2_t(\partial D)$ and $\gamma_T F$ for the tangential trace in $H^{-\frac{1}{2}}(\mathrm{Curl}, \partial D)$ of a vector field in $H(\mathrm{curl}, \Omega)$.

3.1. Perfect conductor

Let E denote the weak solution of the scattering from the perfect conductor D, i.e.

$$\mathcal{A}(E, V) = \ell(V)$$

for all $V \in H_{\mathrm{pc}}(\Omega)$. Let $E_h \in H_{\mathrm{pc}}(\Omega_h)$ denote the weak solution of the scattering problem with respect to the perturbed scatterer D_h, i.e.

$$\int_{\Omega_h} \Big(\mathrm{curl}\, E_h \cdot \overline{\mathrm{curl}\, V_h} - k^2 E_h \cdot \overline{V_h} \Big) \,\mathrm{d}x - \mathrm{i}k \langle \Lambda \gamma_t E_h, \gamma_T V_h \rangle_{\partial B_R(0)} = \ell(V_h) \quad (3.1.1)$$

for all $V_h \in H_{\mathrm{pc}}(\Omega_h)$. Note that only the domain of the volume integral changed. We can not directly compare the solutions E_h and E, since they are in different function spaces. The idea is to use a transformation on $E_h \mapsto \widehat{E_h}$ to arrive at a function $\widehat{E_h} \in H_{\mathrm{pc}}(\Omega)$. This is done by the curl conserving transformation, given by

$$\widehat{E_h}(x) = J_\varphi^\top(x)\widetilde{E_h}(x) = (I + J_h^\top(x))E_h(x + h(x)), \tag{3.1.2}$$

which is used in finite element theory for $H(\mathrm{curl}, \Omega)$, see [39, Section 3.9]. We denote the Jacobian of φ with J_φ. Note, that we have seen this transformation in Section 2.2.2, where we used it to localize vector fields. The curl of $\widehat{E_h}$ and of $\widetilde{E_h}$ with respect to the untransformed coordinates are connected by

$$\mathrm{curl}_\sim \widetilde{E_h} = \frac{1}{\det J_\varphi} J_\varphi \,\mathrm{curl}\, \widehat{E_h} \tag{3.1.3}$$

and we have $E_h \in H(\mathrm{curl}, \Omega_h)$ if and only if $\widehat{E_h} \in H(\mathrm{curl}, \Omega)$, see [39, Corollary 3.58]. This holds also for the space of solutions.

Lemma 3.1. *Let $E_h \in H_{\mathrm{pc}}(\Omega_h)$ and $\widehat{E_h}$ defined by (3.1.2). Then we have $\widehat{E_h} \in H_{\mathrm{pc}}(\Omega)$.*

Proof. We only need to show $\gamma_t \widehat{E_h} = 0$ on ∂D. Let $V_h \in H(\mathrm{curl}, \Omega_h)$. We have by (2.2.4) and applying change of variables $x \mapsto \varphi(x)$

$$\begin{aligned}
\langle \gamma_t \widehat{E_h}, \gamma_T \widehat{V_h}\rangle_{\partial\Omega} &= \int_\Omega \left(\overline{\mathrm{curl}\,\widehat{V_h}} \cdot \widehat{E_h} - \mathrm{curl}\,\widehat{E_h} \cdot \overline{\widehat{V_h}}\right) \mathrm{d}x \\
&= \int_\Omega \left(\frac{1}{\det(J_\varphi)} \overline{\mathrm{curl}\,\widehat{V_h}}^\top J_\varphi^\top J_\varphi^{-\top} \widehat{E_h} - \frac{1}{\det(J_\varphi)}\,\mathrm{curl}\,\widehat{E_h}^\top J_\varphi^\top J_\varphi^{-\top} \overline{\widehat{V_h}}\right) \det(J_\varphi)\,\mathrm{d}x \\
&= \int_\Omega \left(\widetilde{E_h} \cdot \overline{\mathrm{curl}_\sim \widetilde{V_h}} - \mathrm{curl}_\sim \widetilde{E_h} \cdot \overline{\widetilde{V_h}}\right) \det(J_\varphi)\,\mathrm{d}x \\
&= \int_{\Omega_h} \left(\overline{\mathrm{curl}\, V_h} \cdot E_h - \overline{V_h} \cdot \mathrm{curl}\, E\right) \mathrm{d}y = \langle \gamma_t E_h, \gamma_T V_h\rangle_{\partial\Omega_h},
\end{aligned}$$

where $\widehat{V}_h \in H(\mathrm{curl}, \Omega)$ is defined in the same way as $\widehat{E}_h$, i.e.

$$\widehat{V_h} = J_\varphi^\top \widetilde{V_h}.$$

We have $\partial\Omega = \partial D \cup \partial B_R(0)$ and $\partial\Omega_h = \partial D_h \cup \partial B_R(0)$. Note $\gamma_t \widehat{E_h} = \gamma_t E_h$ on $\partial B_R(0)$. Therefore we arrive at

$$\langle \gamma_t \widehat{E_h}, \gamma_T \widehat{V_h}\rangle_{\partial D} = \langle \gamma_t E_h, \gamma_T V_h\rangle_{\partial D_h} = 0$$

for any $V_h \in H(\mathrm{curl}, \Omega_h)$ and therefore $\gamma_t \widehat{E_h} = 0$ on ∂D. $\square$

This allows us to apply the change of variables $x \mapsto \varphi(x)$ to (3.1.1). Together with the transformation (3.1.2), we arrive at the weak formulation for $\widehat{E_h} \in H_{\mathrm{pc}}(\Omega)$, given by

$$\int_\Omega \left(\operatorname{curl} \widehat{E_h}^\top \frac{J_\varphi^\top J_\varphi}{\det(J_\varphi)} \overline{\operatorname{curl} V} - k^2 \widehat{E_h}^\top \det(J_\varphi) J_\varphi^{-1} J_\varphi^{-\top} \overline{V} \right) \mathrm{d}x \\ - \mathrm{i}k \langle \Lambda \gamma_t \widehat{E_h}, \gamma_T V \rangle_{\partial B_R(0)} = \ell(V)$$

for all $V \in H_{\mathrm{pc}}(\Omega)$. We define the bounded sesquilinear form $\mathcal{A}_h : H_{\mathrm{pc}}(\Omega) \times H_{\mathrm{pc}}(\Omega) \to \mathbb{C}$ such that the equation above reads as

$$\mathcal{A}_h(\widehat{E_h}, V) = \ell(V). \tag{3.1.4}$$

To understand the asymptotic behaviour of $\widehat{E_h}$ for $h \to 0$ in C^1, it is important to investigate the coefficients in the weak formulation, which depend on h. The linearizations presented in the following lemma are the main ingredient to prove first continuity and later differentiability of the solution with respect to the perturbation h.

Lemma 3.2. *We have the following asymptotic behavior for $\|h\|_{C^1} \to 0$:*

$$\frac{J_\varphi^\top J_\varphi}{\det(J_\varphi)} = I(1 - \operatorname{div} h) + J_h + J_h^\top + \mathcal{O}(\|h\|_{C^1}^2),$$
$$\det(J_\varphi) J_\varphi^{-1} J_\varphi^{-\top} = I(1 + \operatorname{div} h) - J_h - J_h^\top + \mathcal{O}(\|h\|_{C^1}^2).$$

Proof. Recall $\varphi(x) = x + h(x)$ and therefore we have $J_\varphi = I + J_h$. By

$$(I + J_h)(I - J_h) = (I - J_h)(I + J_h) = I + \mathcal{O}(\|h\|_{C^1}^2)$$

we see $J_\varphi^{-1} = I - J_h + \mathcal{O}(\|h\|_{C^1}^2)$. By the rule of Sarrus, one can see that only the product of the diagonal entries is relevant for the linearization of $\det J_\varphi$ and we arrive at

$$\det(J_\varphi) = \prod_{i=1}^{3} (1 + \partial_{x_i} h_i) + \mathcal{O}(\|h\|_{C^1}^2) = 1 + \operatorname{div} h + \mathcal{O}(\|h\|_{C^1}^2).$$

By considering again

$$(1 + \operatorname{div} h)(1 - \operatorname{div} h) = 1 + \mathcal{O}(\|h\|_{C^1}^2),$$

we conclude

$$\frac{1}{\det(J_\varphi)} = 1 - \operatorname{div} h + \mathcal{O}(\|h\|_{C^1}^2).$$

The claim of the lemma follows by combining these linearizations. □

In the next theorem, we show continuity of the solution with respect to the perturbation $h \in C^1$.

Theorem 3.3. *Let $E \in H_{\mathrm{pc}}(\Omega)$ be the solution of (2.4.4), i.e. a weak solution of the scattering problem from a perfect conductor and $\widehat{E} \in H_{\mathrm{pc}}(\Omega)$ a solution of (3.1.4). Then we have*

$$\lim_{\|h\|_{C^1}\to 0} \|E - \widehat{E_h}\|_{H(\mathrm{curl},\Omega)} = 0.$$

Proof. We consider the bounded linear operators $A, A_h : H_{\mathrm{pc}}(\Omega) \to H_{\mathrm{pc}}(\Omega)$, implicitly defined by the Riesz representation theorem, satisfying

$$\langle AE, V\rangle_{H(\mathrm{curl},\Omega)} = \mathcal{A}(E,V), \quad \langle A_h E, V\rangle_{H(\mathrm{curl},\Omega)} = \mathcal{A}_h(E,V)$$

and let $L \in H(\mathrm{curl},\Omega)$ such that $\ell(V) = \langle L, V\rangle_{H(\mathrm{curl},\Omega)}$. The weak formulations $\mathcal{A}(E,V) = \ell(V)$ and $\mathcal{A}_h(\widehat{E},V) = \ell(V)$ are then equivalent to the operator equations

$$AE = L, \quad A_h\widehat{E_h} = L.$$

We will show convergence of A_h to A in the operator norm. Let $V \in H_{\mathrm{pc}}(\Omega)$. Then we have

$$\begin{aligned}
&\|(A_h - A)V\|^2_{H(\mathrm{curl},\Omega)}\\
&= \langle A_h V, (A_h - AV)\rangle_{H(\mathrm{curl},\Omega)} - \langle AV, (A_h - A)V\rangle_{H(\mathrm{curl},\Omega)}\\
&= \mathcal{A}_h(V, (A_h - A)V) - \mathcal{A}(V, (A_h - A)V)\\
&= \int_\Omega \Big[\operatorname{curl} V^\top \Big(\frac{J_\varphi^\top J_\varphi}{\det(J_\varphi)} - I\Big)\overline{(A_h - A)V}\\
&\qquad - k^2 V^\top\big(\det(J_\varphi)J_\varphi^{-1}J_\varphi^{-\top} - I\big)\overline{(A_h - A)V}\Big]\,\mathrm{d}x.
\end{aligned}$$

By Cauchy-Schwarz and Lemma 3.2 we conclude

$$\|(A_h - A)V\|^2_{H(\mathrm{curl},\Omega)} \leqslant C\|h\|_{C^1}\|V\|_{H(\mathrm{curl},\Omega)}\|(A_h - A)V\|_{H(\mathrm{curl},\Omega)}.$$

and therefore

$$\|A_h - A\| \to 0, \quad \text{for } \|h\|_{C^1} \to 0.$$

Since $\mathcal{A}(E,V) = \ell(V)$ for all $V \in H_{\mathrm{pc}}(\Omega)$ is uniquely solvable with

$$\|E\|_{H(\mathrm{curl},\Omega)} \leqslant C\|\ell\|_{H(\mathrm{curl},\Omega)^\star},$$

see [39, Theorem 10.7], we find A to possess a bounded inverse. With the Perturbation Theorem, see [35, Theorem 10.1], we conclude $\|\widehat{E_h} - E\|_{H(\mathrm{curl},\Omega)} \to 0$ as $\|h\|_{C^1} \to 0$. □

Using the linearizations from Lemma 3.2, we can prove the first differentiability result.

Theorem 3.4. *Let $E \in H_{\mathrm{pc}}(\Omega)$ be the solution of (2.4.4) and $\widehat{E_h} \in H_{\mathrm{pc}}(\Omega)$ of (3.1.4). Then there exists a function $W \in H_{\mathrm{pc}}(\Omega)$, depending linearly and continuously on $h \in C^1$, such that*

$$\lim_{\|h\|_{C^1} \to 0} \frac{1}{\|h\|_{C^1}} \|\widehat{E_h} - E - W\|_{H(\mathrm{curl},\Omega)} = 0.$$

Proof. Motivated by

$$\mathcal{A}(\widehat{E_h} - E, V) = \mathcal{A}(\widehat{E_h}, V) - \ell(V) = \mathcal{A}(\widehat{E_h}, V) - \mathcal{A}_h(\widehat{E_h}, V) \tag{3.1.5}$$

for any $V \in H_{\mathrm{pc}}(\Omega)$ and looking closely at the linearizations, we define $W \in H_{\mathrm{pc}}(\Omega)$ for a given perturbation h as the solution of

$$\begin{aligned}\mathcal{A}(W, V) = \int_\Omega \Big[&\operatorname{curl} E^\top \big(\operatorname{div}(h) I - J_h - J_h^\top\big) \overline{\operatorname{curl} V} \\ &+ k^2 E^\top \big(\operatorname{div}(h) I - J_h - J_h^\top\big) \overline{V} \Big] \,\mathrm{d}x\end{aligned}$$

for all $V \in H_{\mathrm{pc}}(\Omega)$. Using (3.1.5), we calculate

$$\begin{aligned}&\mathcal{A}(\widehat{E_h} - E - W, V) = \mathcal{A}(\widehat{E_h}, V) - \mathcal{A}_h(\widehat{E_h}, V) - \mathcal{A}(W, V) \\ &= \int_\Omega \operatorname{curl} \widehat{E_h}^\top \Big(I - \frac{J_\varphi^\top J_\varphi}{\det(J_\varphi)} - \big(\operatorname{div}(h) I - J_h - J_h^\top\big)\Big) \overline{\operatorname{curl} V} \,\mathrm{d}x \\ &\quad - k^2 \int_\Omega \widehat{E_h}^\top \Big(I - J_\varphi^{-1} J_\varphi^{-\top} \det(J_\varphi) + \big(\operatorname{div}(h) I - J_h - J_h^\top\big)\Big) \overline{V} \,\mathrm{d}x \\ &\quad + \int_\Omega \operatorname{curl}(\widehat{E_h} - E)^\top \Big(\operatorname{div}(h) I - J_h - J_h^\top\Big) \overline{\operatorname{curl} V} \,\mathrm{d}x \\ &\quad + k^2 \int_\Omega (\widehat{E_h} - E)^\top \Big(\operatorname{div}(h) I - J_h - J_h^\top\Big) \overline{\operatorname{curl} V} \,\mathrm{d}x\end{aligned}$$

for any $V \in H_{\mathrm{pc}}(\Omega)$. Using first the linearizations from Lemma 3.2, then applying Cauchy-Schwarz and finally the continuity from Theorem 3.3, we finally conclude

$$\begin{aligned}&\frac{1}{\|h\|_{C^1}} \mathcal{A}(\widehat{E_h} - E - W, V) \\ &\quad \leqslant C\Big(\|\widehat{E_h}\|_{H(\mathrm{curl},\Omega)} \mathcal{O}(\|h\|_{C^1}) + \|\widehat{E_h} - E\|_{H(\mathrm{curl},\Omega)}\Big) \|V\|_{H(\mathrm{curl},\Omega)} \to 0,\end{aligned}$$

as $h \to 0$ in C^1, i.e.

$$\frac{1}{\|h\|_{C^1}} \|\widehat{E_h} - E - W\|_{H(\mathrm{curl}, B_R(0))} \to 0$$

as $h \to 0$ in $C^1(\mathbb{R}^3, \mathbb{R}^3)$. □

The function $W \in H_{\mathrm{pc}}(\Omega)$ is called *material derivative* of E with respect to the perturbation h. Note that W is not a solution of Maxwell's equations. Furthermore, W depends on all values of h in Ω. One would expect a shape derivative to depend only on $h\big|_{\partial D}$. Both issues are solved by considering the so called *domain derivative* E', which is a radiating solution of Maxwell's equations and depends only on $h\big|_{\partial D}$. The domain derivative can be extracted from W. We introduce the notation $E(x,h) = E_h(x)$ and set $E(x,0) = E(x)$. To motivate the following theorem, consider the formal Taylor expansion

$$\begin{aligned}
\widehat{E_h}(x) &= \big(I + J_h^\top(x)\big)E_h(x + h(x)) = \big(I + J_h^\top(x)\big)E(x + h(x), h) \\
&= \big(I + J_h^\top(x)\big)\Big(E(x,0) + J_E(x)h(x) + \frac{\mathrm{d}}{\mathrm{d}h}E(x) + \mathcal{O}(\|h\|_{C^1}^2)\Big) \\
&= E(x) + \frac{\mathrm{d}}{\mathrm{d}h}E(x) + J_E(x)h(x) + J_h^\top(x)E(x) + \mathcal{O}(\|h\|_{C^1}^2). \qquad (3.1.6)
\end{aligned}$$

In the previous theorem, we formally derived

$$W = \frac{\mathrm{d}}{\mathrm{d}h}\widehat{E_h}.$$

This motivates the definition $E' = \frac{\mathrm{d}}{\mathrm{d}h}E = W - J_h^\top E - J_E h$. The next theorem shows, that this is the right choice to define the domain derivative E'. This decomposition requires additional regularity of the boundary, since we need higher regularity of our solutions. First, we show the following lemma.

Lemma 3.5. *Let ∂D be of class C^{m+1} for some $m \in \mathbb{N}$. Any weak solution $(E, H) \in H_{\mathrm{pc}}(\Omega) \times H(\mathrm{curl}, \Omega)$ of the scattering from a perfect conductor satisfies $(E, H) \in H^m(\Omega, \mathbb{C}^3) \times H^m(\Omega, \mathbb{C}^3)$.*

Proof. The proof is an application of [1, Corollary 2.15]. They show, that if ∂D is of class C^{m+1} for some integer $m \in \mathbb{N}$, the spaces

$$\begin{aligned}
\{E \in L^2(\Omega, \mathbb{C}^3) :\ \mathrm{curl}\, E \in & H^{m-1}(\Omega, \mathbb{C}^3), \\
& \mathrm{div}\, E \in H^{m-1}(\Omega) \,\text{and}\, \nu \times E \in H^{m-\frac{1}{2}}(\partial D, \mathbb{C}^3)\}, \\
\{E \in L^2(\Omega, \mathbb{C}^3) :\ \mathrm{curl}\, E \in & H^{m-1}(\Omega, \mathbb{C}^3), \\
& \mathrm{div}\, E \in H^{m-1}(\Omega) \,\text{and}\, \nu \cdot E \in H^{m-\frac{1}{2}}(\partial D)\}
\end{aligned}$$

are both continuously embedded in $H^m(\Omega, \mathbb{C}^3)$. First, we observe $\operatorname{div} E = \operatorname{div} H = 0 \in L^2(\Omega, \mathbb{C}^3)$ by Maxwell's equations. By the boundary condition $\gamma_t E = 0$, we immediately conclude $E \in H^1(\Omega, \mathbb{C}^3)$ since E is an element of the first space. Again by the boundary condition, we have

$$H \cdot \nu = \frac{1}{\mathrm{i}k} \operatorname{curl} E \cdot \nu = \frac{1}{\mathrm{i}k} \operatorname{Div}_{\partial D}(E \times \nu) = 0,$$

see (2.2.6), i.e. $H \in H^1(\Omega, \mathbb{C}^3)$ since H is an element of the second space. Now, we have $\operatorname{curl} E, \operatorname{curl} H \in H^1(\Omega, \mathbb{C}^3)$ by Maxwell's equations. We can repeat the argument and conclude $E, H \in H^2(\Omega, \mathbb{C}^3)$. By induction we conclude $E, H \in H^m(\Omega, \mathbb{C}^3)$. □

Now we can prove the decomposition of the material derivative.

Theorem 3.6. *Let ∂D be of class C^2. In the setting of Theorem 3.4, we have $E' = W - J_h^\top E - J_E h \in H(\operatorname{curl}, \Omega)$. E' can be uniquely extended to the radiating weak solution of Maxwell's equations*

$$\operatorname{curl} E' - \mathrm{i}k\, H' = 0, \quad \operatorname{curl} H' + \mathrm{i}k\, E' = 0$$

in $\mathbb{R}^3 \setminus \overline{D}$ with boundary condition

$$\nu \times E' = \overrightarrow{\operatorname{Curl}}_{\partial D}(h_\nu E_\nu) - \mathrm{i}k h_\nu \gamma_T H \quad \text{on } \partial D. \tag{3.1.7}$$

Proof. We define $E' = W - J_h^\top E - J_E h$. Since the boundary ∂D is of class C^2, we have E, H in $H^1(\Omega)$ with vanishing tangential trace of the electric field by Lemma 3.5. By the Trace Theorem 2.4, we have $E\big|_{\partial D} \in H^{\frac{1}{2}}(\partial D, \mathbb{C}^3)$. The normal vector field is in $C^1(\partial D, \mathbb{S}^2)$ and therefore $E_\nu = E \cdot \nu \in H^{\frac{1}{2}}(\partial D)$. By Theorem 2.6 we have $\overrightarrow{\operatorname{Curl}}_{\partial D}(h_\nu E_\nu) \in H^{-\frac{1}{2}}(\operatorname{Div}, \partial D)$. Since $H \in H^1(\Omega)$, we have also $\gamma_T H \in H^{-\frac{1}{2}}(\operatorname{Div}, \partial D)$. We conclude, that the boundary condition is well defined for $E' \in H(\operatorname{curl}, \Omega)$. Since $E \in H^1(\Omega, \mathbb{C}^3)$, we have $E' = W - J_h^\top E - J_E h \in L^2(\Omega, \mathbb{C}^3)$. Some basic vector calculus shows

$$\begin{aligned}\operatorname{curl}(J_h^\top E + J_E h) &= \operatorname{curl}\big((J_E - J_E^\top)h + \nabla(h^\top E)\big) \\ &= \operatorname{curl}(\operatorname{curl} E \times h) = \operatorname{div}(h) \operatorname{curl} E + J_{\operatorname{curl} E} - J_h \operatorname{curl} E.\end{aligned} \tag{3.1.8}$$

Note that $H = \frac{1}{\mathrm{i}k} \operatorname{curl} E \in H^1(\Omega, \mathbb{C}^3)$ and therefore $\operatorname{curl} E' \in L^2(\Omega, \mathbb{C}^3)$. So we conclude $E' \in H(\operatorname{curl}, \Omega)$. Since $\nu \times W = 0$ on ∂D, we find

$$\begin{aligned}\nu \times E' &= -\nu \times (J_E h + J_h^\top E) = -\nu \times (J_E h - J_E^\top h) - \nu \times (J_h^\top E + J_E^\top h) \\ &= -\nu \times (\operatorname{curl} E \times h) - \nu \times \nabla(h^\top E).\end{aligned}$$

Since $\nu \times E = 0$ and with $\nu \times \nabla = \nu \times \operatorname{Grad}_{\partial D} = -\overrightarrow{\operatorname{Curl}}_{\partial D}$ on ∂D we have

$$-\nu \times \nabla(h^\top E) = \overrightarrow{\operatorname{Curl}}(h_\nu E_\nu).$$

Furthermore, we have $\nu \times (\operatorname{curl} E \times h) = \mathrm{i}k\big(\nu \times (H \times h)\big)$. Using $a \times (b \times c) = (a \cdot c)b - (a \cdot b)c$ and the decomposition of h and H into normal and tangential component, we find

$$\nu \times (\operatorname{curl} E \times h) = \mathrm{i}k(h_\nu H_\tau + H_\nu h_\tau).$$

From (2.2.6) with $F = E$ we find $H_\nu = 0$ and therefore conclude the boundary condition

$$\nu \times E' = \overrightarrow{\operatorname{Curl}}_{\partial D}(h_\nu E_\nu) - \mathrm{i}k h_\nu \gamma_T H. \tag{3.1.9}$$

To see that E', together with $H' = \frac{1}{\mathrm{i}k} \operatorname{curl} E'$ is a radiating solution of Maxwell's equation, we start by noticing

$$\begin{aligned}
\mathcal{A}(F, V) &= \int_\Omega \Big(\operatorname{curl} F^\top \overline{\operatorname{curl} V} - k^2 F^\top \overline{V}\Big)\,\mathrm{d}x - \mathrm{i}k\langle \Lambda(\gamma_t F), \gamma_T V\rangle_{\partial B_R(0)} \\
&= \int_\Omega (\operatorname{curl}^2 F - k^2 F)^\top \overline{V}\,\mathrm{d}x - \mathrm{i}k\langle \Lambda(\gamma_t F) - \gamma_t G, V\rangle_{\partial B_R(0)} = 0,
\end{aligned}$$

for any pair of radiating solutions (F, G) of Maxwell's equations and any $V \in H_{\mathrm{pc}}(\Omega)$, since $\Lambda(\gamma_t F) = \gamma_t G$ and $\nu \times V = 0$ on ∂D. Therefore, since we already have shown the boundary condition (3.1.9), we only need to show

$$\mathcal{A}(E', V) = \mathcal{A}(W - J_h^\top E - J_E h, V) = 0$$

for any $V \in H_{\mathrm{pc}}(\Omega)$. Let $V \in H_{\mathrm{pc}}(\Omega)$. Then

$$\begin{aligned}
&\mathcal{A}(W, V) - \mathcal{A}(J_h^\top E + J_E h, V) \\
&= \int_\Omega \Big(\operatorname{curl} E^\top \big(\operatorname{div}(h) I - J_h - J_h^\top\big)\overline{\operatorname{curl} V} + k^2 E^\top \big(\operatorname{div}(h) I - J_h - J_h^\top\big)\overline{V}\Big)\,\mathrm{d}x \\
&\qquad - \int_\Omega \Big(\operatorname{curl}(J_h^\top E + J_E h)^\top \overline{\operatorname{curl} V} - k^2 (J_h^\top E + J_E h)^\top \overline{V}\Big)\,\mathrm{d}x.
\end{aligned}\tag{3.1.10}$$

Using again (3.1.8), we find

$$\begin{aligned}
&\mathcal{A}(W, V) - \mathcal{A}(J_h^\top E + J_E h, V) \\
&\qquad = k^2 \int_\Omega \Big(J_E h + \operatorname{div}(h) E - J_h E\Big)^\top \overline{V}\,\mathrm{d}x \\
&\qquad\qquad - \int_\Omega \Big(J_{\operatorname{curl} E} h + J_h^\top \operatorname{curl} E\Big)^\top \overline{\operatorname{curl} V}\,\mathrm{d}x.
\end{aligned}$$

From $\operatorname{div} E = 0$ in $\mathbb{R}^3 \setminus \overline{D}$, we conclude

$$\operatorname{curl}(E \times h) = \operatorname{div}(h)E + J_E h - J_h E$$

and therefore

$$\begin{aligned}
&\mathcal{A}(W,V) - \mathcal{A}(J_h^\top E + J_E h, V) \\
&\qquad = k^2 \int_\Omega \operatorname{curl}(E \times h)^\top \overline{V}\,\mathrm{d}x - \int_\Omega \Big(J_{\operatorname{curl} E} h + J_h^\top \operatorname{curl} E\Big)^\top \overline{\operatorname{curl} V}\,\mathrm{d}x.
\end{aligned}$$

With Maxwell's equations we compute the identity

$$\begin{aligned}
&J_{\operatorname{curl} E} h + J_h^\top \operatorname{curl} E = \big(J_{\operatorname{curl} E} - J_{\operatorname{curl} E}^\top\big)h + J_{\operatorname{curl} E}^\top h + J_h^\top E \\
&\qquad = \big(\operatorname{curl}\operatorname{curl} E\big) \times h + \nabla(h^\top \operatorname{curl} E) = k^2\big(E \times h\big) + \nabla(h^\top \operatorname{curl} E).
\end{aligned}$$

Together with

$$\operatorname{div}\big((E \times h) \times \overline{V}\big) = \operatorname{curl}(E \times h)^\top \overline{V} - (E \times h)\overline{\operatorname{curl} V}$$

we conclude

$$\begin{aligned}
&\mathcal{A}(W,V) - \mathcal{A}(J_h^\top E + J_E h, V) \\
&\qquad = k^2 \int_\Omega \operatorname{div}\big((E \times h) \times \overline{V}\big)\,\mathrm{d}x - \int_\Omega \nabla(h^\top \operatorname{curl} E)^\top \overline{\operatorname{curl} V}\,\mathrm{d}x \\
&\qquad\qquad = \int_\Omega \operatorname{div}\Big[k^2\big(E \times h\big) \times \overline{V} - (h^\top \operatorname{curl} E)\overline{\operatorname{curl} V}\Big]\,\mathrm{d}x.
\end{aligned}$$

Since h is compactly supported in $B_R(0)$, we have $h \equiv 0$ on $\partial B_R(0)$. We apply the divergence theorem in Ω to the right hand side of the last equation and get

$$\begin{aligned}
&\mathcal{A}(W,V) - \mathcal{A}(J_h^\top E + J_E h, V) \\
&\qquad = \int_{\partial D} \Big((h^\top \operatorname{curl} E)(\nu^\top \overline{\operatorname{curl} V}) - k^2\big((E \times h) \times \overline{V}\big)^\top \nu\Big)\,\mathrm{d}s.
\end{aligned}$$

Note the sign change, since ν outwards drawn normal vector to D. The first term vanishes, since

$$\nu^\top \overline{\operatorname{curl} V} = \operatorname{Curl}_{\partial D} \overline{V} = \operatorname{Div}_{\partial D}(\overline{V} \times \nu) = 0,$$

see (2.2.6) and since $V \in H_{\mathrm{pc}}(\Omega)$ has vanishing tangential trace on ∂D. For the second term, we compute

$$\big((E\times h)\times \overline{V}\big)\cdot \nu = (E\cdot \overline{V})(h\cdot\nu) - (\overline{V}\cdot h)(E\cdot\nu) = (h\times E)\cdot(\nu\times\overline{V}) = 0$$

and therefore conclude

$$\mathcal{A}(E', V) = \mathcal{A}(W, V) - \mathcal{A}(J_h^\top E + J_E h, V) = 0$$

for all $V \in H_{\mathrm{pc}}(\Omega)$, which finishes the proof. □

3.1.1. The second domain derivative

In this section, we present the characterization of the second domain derivative of the perfect conductor. Some difficulties arise, which can be treated successfully in the same way as in the case of acoustic scattering, see [27]. We will present the procedure. The first observation is the following: Considering two small variations h_1, h_2 with compact support in $B_R(0)$, we arrive at the perturbed boundary

$$(\partial D_{h_2})_{h_1} = \{y = \varphi_1(\varphi_2(x)) = x + h_2(x) + h_1(x + h_2(x)) : x \in \partial D\}.$$

This variation is not symmetric in h_1 and h_2, a property one expects from a second derivative, see [17, Chapter VIII.12]. Let $E_i'[\partial D]$ be the domain derivative of the perfect conductor with respect to the variation h_i, $i = 1, 2$ and the scatterer ∂D. Our goal is to find a radiating solution of Maxwell's equations E'', depending continuously on h_1 and h_2, being symmetric with respect to h_1 and h_2, satisfying

$$\lim_{\|h_2\|\to 0} \frac{1}{\|h_2\|} \sup_{\|h_1\|=1} \left\| E'_{h_1\circ\varphi_2^{-1}}[\partial D_{h_2}] - E'_{h_1}[\partial D] - E'' \right\| = 0.$$

Together with the Taylor expansion

$$h_1 \circ \varphi_2^{-1} = h_1 - J_{h_1} h_2 + \mathcal{O}(\|h_2\|^2)$$

we arrive at the characterization

$$E'' = (E_1')_2' - E_h' \tag{3.1.11}$$

with $h = J_{h_1} h_2$. We dropped the dependency of the scatterer, since all terms are with respect to ∂D. The first term on the right hand side of (3.1.11) is the domain derivative with respect to the variation h_2 of the domain derivative with respect to the variation h_1. This is the unknown function, which we have to determine. The second term E_h' is the previous calculated domain derivative with respect to the variation $h = J_{h_1} h_2$. In this section, we will prove the existence of E'' and provide a characterization, which highlights the symmetry of E'' with respect to h_1 and h_2.

Let $W_i \in H(\mathrm{curl}, \Omega)$ denote the material derivative of the perfect conductor ∂D with respect to the variation h_i, $i = 1, 2$. Recall the weak formulation

$$\begin{aligned} \mathcal{A}(W_i, V) &= \int_\Omega \left(\mathrm{curl}\, E^\top \overline{\mathrm{curl}\, V} - k^2 E^\top \overline{V} \right) \mathrm{d}x + \mathrm{i}k \langle \Lambda(\nu \times E), V \rangle_{|x|=R} \\ &= \int_\Omega \left(\mathrm{curl}\, E^\top A_i \overline{\mathrm{curl}\, V} + k^2 E^\top A_i \overline{V} \right) \mathrm{d}x, \end{aligned} \tag{3.1.12}$$

where we used the abbreviation A_i for the symmetric matrix given by

$$A_i = \mathrm{div}(h_i) I - J_{h_i} - J_{h_i}^\top.$$

As before we denote by $\widetilde{W_1} \in H(\mathrm{curl}, \Omega_{h_2})$ the solution of (3.1.12) with Ω_{h_2} instead of Ω. We define

$$\widehat{W}_{1,h_2} = J_{\varphi_2}^\top \widetilde{W_1} \in H_{\mathrm{pc}}(\Omega)$$

The function $\widehat{W}_{1,h_2}$ solves

$$\begin{aligned} &\int_\Omega \left(\mathrm{curl}\, \widehat{W}_{1,h_2}^\top \Big(\frac{J_{\varphi_2}^\top J_{\varphi_2}}{\det J_{\varphi_2}} \Big) \overline{\mathrm{curl}\, V} - k^2 \widehat{W}_{1,h_2}^\top \Big(\det(J_{\varphi_2}) J_{\varphi_2}^{-1} J_{\varphi_2}^{-\top} \Big) \overline{V} \right) \mathrm{d}x \\ &\qquad\qquad + \mathrm{i}k \langle \Lambda(\nu \times \widehat{W}_{1,h_2}), V \rangle_{|x|=R} \\ &= \int_\Omega \left(\mathrm{curl}\, \widehat{E}_{h_2}^\top \Big(\frac{J_{\varphi_2}^\top \widetilde{A_1} J_{\varphi_2}}{\det J_{\varphi_2}} \Big) \,\mathrm{curl}\, V + k^2 \widehat{E}_{h_2} \Big(\det(J_{\varphi_2}) J_{\varphi_2}^{-1} \widetilde{A_1} J_{\varphi_2}^{-\top} \Big) \overline{V} \right) \mathrm{d}x. \end{aligned} \tag{3.1.13}$$

Note that in contrast to the first domain derivative, we had to transform the right hand side as well. Again, we have used the notation

$$\widetilde{A_1}(x) = A_1(\varphi_2(x)) = A_1(x + h_2(x)).$$

We need the following lemma, which characterizes the linearizations of the new matrices in the equation above.

Lemma 3.7. *Let $A \in C^1(\mathbb{R}^3, \mathbb{R}^{3\times 3})$ and $\varphi(x) = x + h(x)$ with $h \in C^1$ sufficiently small. Then we have*

$$\frac{J_\varphi^\top \widetilde{A} J_\varphi}{\det J_\varphi} = A + J_h^\top A + A J_h - \mathrm{div}(h) A + A'(h) + \mathcal{O}(\|h\|_{C^1}^2),$$

$$\det(J_\varphi) J_\varphi^{-1} \widetilde{A} J_\varphi^{-\top} = A - J_h A - A J_h^\top + \operatorname{div}(h) A + A'(h) + \mathcal{O}(\|h\|_{C^1}^2),$$

where the matrix $A'(h) \in C(\mathbb{R}^3, \mathbb{R}^{3\times 3})$ *is given by* $(A'(h))_{ij} = h^\top \nabla A_{ij}$, $i, j = 1, \ldots, 3$.

Proof. The linearization follows from combining the linearizations in Lemma 3.2 and the Taylor expansion

$$A_{ij}(x + h(x)) = A_{ij}(x) + h^\top \nabla A_{ij}(x) + \mathcal{O}(\|h\|_{C^1}^2)$$

for the coefficients of the matrix A. □

With this Lemma, we can proof continuity of $\widehat{W}_{1,h_2}$ with respect to h_2.

Theorem 3.8. *Let* $W_1 \in H_{\mathrm{pc}}(\Omega)$ *be the solution of (3.1.12) and* $\widehat{W}_{1,h_2} \in H_{\mathrm{pc}}(\Omega)$ *a solution of (3.1.13). Then we have*

$$\lim_{\|h_2\|_{C^1} \to 0} \|W_1 - \widehat{W}_{1,h_2}\|_{H(\mathrm{curl},\Omega)} = 0.$$

Proof. The proof is done very similar as in Theorem 3.3 with the additional consideration of the linearization of the right hand side. Let $\ell_{h_1}(V)$ denote the right hand side of (3.1.12) with $i = 1$ and let $\ell_{h_2,h_1}(V)$ denote the right hand side of (3.1.13). Recall the notation $\mathcal{A}_{h_2}$ for the sesquilinear form, such that the left hand side of (3.1.13) is given by $\mathcal{A}_{h_2}(\widehat{W}_{1,h_2}, V)$. Then we have

$$\begin{aligned}\mathcal{A}(\widehat{W}_{1,h_2} - W_1, V) = \mathcal{A}(\widehat{W}_{1,h_2}, V) - \mathcal{A}_{h_2}(\widehat{W}_{1,h_2}, V) + \ell_{h_1,h_2}(V) - \ell_{h_2}(V) \\ \pm \int_\Omega \Big(\operatorname{curl} \widehat{E}_{h_2}^\top A_1 \operatorname{curl} V + k^2 \widehat{E}_{h_2}^\top A_1 \overline{V} \Big) \,\mathrm{d}x.\end{aligned}$$

This leads to

$$\begin{aligned}&\mathcal{A}(\widehat{W}_{1,h_2} - W_1, V) \\ &= \int_\Omega \Bigg(\operatorname{curl} \widehat{W}_{1,h_2} \Big(I - \frac{J_{\varphi_2}^\top J_{\varphi_2}}{\det J_{\varphi_2}} \Big) \operatorname{curl} V \\ &\qquad - k^2 \widehat{W}_{1,h_2}^\top \Big(I - \det J_{\varphi_2} J_{\varphi_2}^{-1} J_{\varphi_2}^{-\top} \Big) \overline{V} \Bigg) \,\mathrm{d}x \\ &\quad + \int_\Omega \Bigg(\operatorname{curl} \widehat{E}_{h_2}^\top \Big(\frac{J_{\varphi_2}^\top \widetilde{A_1} J_{\varphi_2}}{\det J_{\varphi_2}} - A_1 \Big) \overline{\operatorname{curl} V} \\ &\qquad + k^2 \widehat{E}_{h_2}^\top \Big(\det J_{\varphi_2} J_{\varphi_2}^{-1} \widetilde{A_1} J_{\varphi_2}^{-\top} - A_1 \Big) \overline{V} \Bigg) \,\mathrm{d}x\end{aligned}$$

$$+\int_\Omega \left(\operatorname{curl}(\widehat{E}_{h_2}^\top - E)^\top A_1 \overline{\operatorname{curl} V} + k^2 (\widehat{E}_{h_2} - E)^\top A_1 \overline{V} \right) \mathrm{d}x.$$

By Lemma 3.7 and Theorem 3.3, we conclude

$$\mathcal{A}(\widehat{W}_{1,h_2} - W_1, V) \to 0, \quad h_2 \to 0 \quad \text{in } C^1.$$

By again a perturbation argument, we conclude

$$\lim_{\|h\|_{C^1}\to 0} \|\widehat{W}_{1,h_2} - W_1\|_{H(\operatorname{curl},\Omega)} = 0.$$

□

We prove differentiability of $\widehat{W}_{1,h_2} \in H(\operatorname{curl},\Omega)$ with respect to $h_2 \in C^1$.

Theorem 3.9. *Let $W_1 \in H_{\mathrm{pc}}(\Omega)$ be the solution of (3.1.12) and $\widehat{W}_{1,h_2} \in H_{\mathrm{pc}}(\Omega)$ of (3.1.13). Then there exists a function $W_1' \in H_{\mathrm{pc}}(\Omega)$, depending linear and continuous on $h_2 \in C^1$, such that*

$$\lim_{\|h_2\|_{C^1}\to 0} \frac{1}{\|h_2\|_{C^1}} \|\widehat{W}_{1,h_2} - W_1 - W_1'\|_{H(\operatorname{curl},\Omega)} = 0.$$

Proof. By considering Lemma 3.7 and observing the differences occurring in the proof of the previous theorem, we define $W_1' \in H_{\mathrm{pc}}(\Omega)$ as the solution of

$$\begin{aligned}
\mathcal{A}(W_1', V) = &\int_\Omega \left(\operatorname{curl} W_1^\top A_2 \overline{\operatorname{curl} V} + k^2 W_1^\top A_2 \overline{V} \right) \mathrm{d}x \\
&+ \int_\Omega \left(\operatorname{curl} W_2^\top A_1 \overline{V} + k^2 W_2^\top A_1 \overline{V} \right) \mathrm{d}x \\
&+ \int_\Omega \operatorname{curl} E^\top \Big(J_{h_2}^\top A_1 + A_1 J_{h_2} - \operatorname{div}(h_2) A_1 + A_1'(h_2) \Big) \overline{\operatorname{curl} V} \, \mathrm{d}x \\
&+ k^2 \int_\Omega E^\top \Big(- J_{h_2} A_1 - A_1 J_{h_2}^\top + \operatorname{div}(h_2) A_1 + A_1'(h_2) \Big) \overline{V} \, \mathrm{d}x.
\end{aligned}$$

We consider the difference $\mathcal{A}(\widehat{W}_{1,h_2} - W_1 - W_1', V)$ and add some smart zeros. This leads to

$$\begin{aligned}
&\mathcal{A}(\widehat{W}_{1,h_2} - W_1 - W_1', V) \\
&= \mathcal{A}(\widehat{W}_{1,h_2}, V) - \mathcal{A}_{h_2}(\widehat{W}_{1,h_2}, V) + \ell_{h_1,h_2}(V) - \mathcal{A}(W_1, V) - \mathcal{A}(W_1', V) \\
&\quad \pm \int_\Omega \left(\widehat{W}_{1,h_2} A_2 \overline{\operatorname{curl} V} - k^2 \widehat{W}_{1,h_2} A_2 \overline{V} \right) \mathrm{d}x
\end{aligned}$$

$$
\begin{aligned}
&\pm \int_\Omega \Big(\operatorname{curl} \widehat{E}_{h_2}^\top A_1 \overline{\operatorname{curl} V} + k^2 \widehat{E}_{h_2}^\top A_1 \overline{V}\Big)\,\mathrm{d}x \\
&\pm \int_\Omega \operatorname{curl} \widehat{E}_{h_2}^\top \Big(J_{h_2}^\top A_1 + A_1 J_{h_2} - \operatorname{div}(h_2) A_1 + A_1'(h_2)\Big)\,\mathrm{d}x \\
&\pm k^2 \int_\Omega \widehat{E}_{h_2}^\top \Big(- J_{h_2} A_1 - A_1 J_{h_2}^\top + \operatorname{div}(h_2) A_1 + A_1'(h_2)\Big)\overline{V}\,\mathrm{d}x.
\end{aligned}
$$

We gather the terms, such that we can apply Cauchy-Schwarz, the linearization Lemmata 3.2 and 3.7, and Theorem 3.3 by

$$
\begin{aligned}
&\mathcal{A}(\widehat{W}_{1,h_2} - W_1 - W_1', V) \\
&= \int_\Omega \operatorname{curl} \widehat{W}_{1,h_2} \Big(I - \frac{J_{\varphi_2}^\top J_{\varphi_2}}{\det J_{\varphi_2}} - A_2\Big) \operatorname{curl} V \,\mathrm{d}x \\
&\quad - k^2 \int_\Omega \widehat{W}_{1,h_2}^\top \Big(I - \det J_{\varphi_2} J_{\varphi_2}^{-1} J_{\varphi_2}^{-\top} + A_2\Big)\overline{V}\,\mathrm{d}x \\
&\quad + \int_\Omega \Big(\operatorname{curl}(\widehat{W}_{1,h_2} - W_1)^\top A_2 \overline{\operatorname{curl} V} - k^2 (\widehat{W}_{1,h_2} - W_1)^\top A_2 \overline{V}\Big)\,\mathrm{d}x \\
&\quad + \int_\Omega \operatorname{curl} \widehat{E}_{h_2}^\top \Big(\frac{J_{\varphi_2}^\top \widetilde{A_1} J_{\varphi_2}}{\det J_{\varphi_2}} - A_1 - J_{h_2}^\top A_1 \\
&\qquad\qquad - A_1 J_{h_2} + \operatorname{div}(h_2) I - A_1'(h_2)\Big)\overline{\operatorname{curl} V}\,\mathrm{d}x \\
&\quad + k^2 \int_\Omega \widehat{E}_{h_2}^\top \Big(\det(J_{\varphi_2}) J_{\varphi_2}^{-1} \widetilde{A_1} J_{\varphi_2}^{-\top} - A_1 \\
&\qquad\qquad + J_{h_2} A_1 + A_1 J_{h_2}^\top - \operatorname{div}(h_2) I - A_1'(h_2)\Big)\overline{V}\,\mathrm{d}x \\
&\quad + \int_\Omega \Big(\operatorname{curl}\big(\widehat{E}_{h_2} - E - W_2\big)^\top A_1 \overline{\operatorname{curl} V} + k^2 (\widehat{E}_{h_2} - E - W_2)^\top A_1 \overline{V}\Big)\,\mathrm{d}x \\
&\quad + \int_\Omega \operatorname{curl}\big(\widehat{E}_{h_2} - E\big)^\top \Big(J_{h_2}^\top A_1 + A_1 J_{h_2} - \operatorname{div}(h_2) A_1 + A_1'(h_2)\Big)\overline{\operatorname{curl} V}\,\mathrm{d}x \\
&\quad + k^2 \int_\Omega \big(\widehat{E}_{h_2} - E\big)^\top \Big(- J_{h_2} A_1 - A_1 J_{h_2}^\top + \operatorname{div}(h_2) A_1 + A_1'(h_2)\Big)\overline{V}\,\mathrm{d}x.
\end{aligned}
$$

This leads finally with some constant $C > 0$ to

$$
\begin{aligned}
&\mathcal{A}(\widehat{W}_{1,h_2} - W_1 - W_1', V) \\
&\quad \leqslant C\Big(\|\widehat{W}_{1,h_2}\| \mathcal{O}(\|h_2\|_{C^1}^2) + \|\widehat{W}_{1,h_2} - W_1\| \mathcal{O}(\|h_2\|_{C^1}) \\
&\qquad + \|\widehat{E}_{h_2}\| \mathcal{O}(\|h_2\|_{C^1}^2) + o(\|h_2\|_{C^1}) + \|\widehat{E}_{h_2} - E\| \mathcal{O}(\|h_2\|_{C^1})\Big)\|V\|,
\end{aligned}
$$

where the non specified norms are always the $H(\mathrm{curl},\Omega)$-norm. Again by a perturbation argument, we conclude

$$\lim_{\|h_2\|_{C^1}\to 0} \frac{1}{\|h_2\|_{C^1}} \|\widehat{W}_{1,h_2} - W_1 - W_1'\|_{H(\mathrm{curl},\Omega)} = 0.$$

□

Note that $W_1' \in H_{\mathrm{pc}}(\Omega)$ is the material derivative with respect to h_2 of the material derivative with respect to h_1 and contains by linearity the domain derivative with respect to h_2 of the domain derivative with respect to h_1, noted by $(E_1')_2'$. Similar to the first domain derivative, we consider the formal Taylor expansion of $\widehat{W}_{1,h_2}$:

$$\begin{aligned}
&\widehat{W}_{1,h_2}(x) = (I + J_{h_2}^\top(x))W_{1,h_2}(x + h_2(x)) \\
&= (I + J_{h_2}^\top(x))W_1(x + h_2(x), h_2) \\
&= \big(I + J_{h_2}^\top(x)\big)\Big(W_1(x,0) + J_{W_1}(x)h_2(x) + \frac{\mathrm{d}}{\mathrm{d}h_2}W_1(x) + \mathcal{O}(\|h_2\|^2)\Big).
\end{aligned}$$

With $W_1 = E_1' + J_{h_1}^\top E + J_E h_1$ we have

$$\frac{\mathrm{d}}{\mathrm{d}h_2}W_1 = (E_1')_2' + J_{h_1}^\top E_2' + J_{E_2'}h_1.$$

We have formally calculated

$$W_1' = \frac{\mathrm{d}}{\mathrm{d}h_2}\widehat{W}_{1,h_2}.$$

This motivates the Ansatz

$$(E_1')_2' = W_1' - J_{h_2}^\top W_1 - J_{W_1}h_2 - J_{h_1}^\top E_2' - J_{E_2'}h_1,$$

which will be proven in the next theorem. Similar to the first domain derivative, this decomposition holds only, if we assume higher regularity of the boundary.

Theorem 3.10. *Let ∂D be regular. In the setting of Theorem 3.9, let*

$$(E_1')_2' = W_1' - J_{h_2}^\top W_1 - J_{W_1}h_2 - J_{h_1}^\top E_2' - J_{E_2'}h_1.$$

Then $(E_1')_2' \in H(\mathrm{curl},\Omega)$ is a radiating solution of Maxwell's equations.

Proof. Similar to the proof of the first domain derivative, we define $(E_1)_2'$ by the right hand side of equation stated in the theorem, i.e.

$$(E_1')_2' = W_1' - J_{h_2}^\top W_1 - J_{W_1} h_2 - J_{h_1}^\top E_2' - J_{E_2'} h_1,$$

which defines by Lemma 3.5 a function in $H(\operatorname{curl}, \Omega)$. Note, that the proof of Lemma 3.5 shows, that a sufficiently smooth solution (E, H) to the scattering problem implies also high regularity of the domain derivative E' and therefore also high regularity of the material derivative W.

To see, that this is a radiating solution of Maxwell's equations, we will show $\mathcal{A}\big((E_1')_2', V\big) = 0$ for all $V \in H(\operatorname{curl}, \Omega)$. Since the material derivatives W_i, $i = 1, 2$ do not satisfy Maxwell's equations, we want to remove them from the above expression. We have

$$W_i = E_i' + J_{h_i}^\top E + J_E h_i = E_i' + \nabla(h_i^\top E) + \operatorname{curl} E \times h_i.$$

From this, we can calculate the curl of the material derivative by

$$\begin{aligned}
\operatorname{curl} W_i &= \operatorname{curl} E_i' + \operatorname{curl}\big(\operatorname{curl} E \times h_i\big) \\
&= \operatorname{curl} E_i' + \operatorname{curl} E \operatorname{div}(h_i) + \big(J_{\operatorname{curl} E} - J_{\operatorname{curl} E}^\top\big) h_i \\
&\qquad + \big(J_{\operatorname{curl} E}^\top h_i + J_{h_i}^\top \operatorname{curl} E\big) - \big(J_{h_i} + J_{h_i}^\top\big) \operatorname{curl} E \\
&= \operatorname{curl} E_i' + A_i \operatorname{curl} E + k^2 (E \times h_i) + \nabla(h_i^\top \operatorname{curl} E).
\end{aligned}$$

In the proof for the first domain derivative, we have shown, that if $F \in H^1(\Omega, \mathbb{C}^3)$ is a solution of Maxwell's equations, i.e. $\operatorname{div} F = 0$ and $\operatorname{curl}^2 F - k^2 F = 0$, then we have for any $V \in H_{\mathrm{pc}}(\Omega)$ and $i = 1, 2$

$$\int_\Omega \Big(\operatorname{curl} F^\top A_i \overline{V} + k^2 F^\top A_i \overline{V}\Big)\,\mathrm{d}x - \mathcal{A}(J_{h_i}^\top F + J_F h_i, V) = 0. \tag{3.1.14}$$

Note, that we did not use the boundary condition of $\nu \times E = 0$ in the proof but only $\nu \times V = 0$. Therefore, we can apply (3.1.14) with $F = E_j'$ and $i \neq j$, i.e. we have

$$\int_\Omega \Big(\operatorname{curl} E_j'^\top A_i \overline{V} + k^2 E_j'^\top A_i \overline{V}\Big)\,\mathrm{d}x - \mathcal{A}(J_{h_i}^\top E_j' + J_{E_j'} h_i, V) = 0$$

for $i, j = 1, 2$, $i \neq j$. In order to eliminate W_1 from the terms we subtracted from $(E_1')_2'$ in the definition, we consider

$$J_{h_2}^\top W_1 + J_{W_1} h_2 = J_{h_2}^\top E_1' + J_{E_1'} h_2 + J_{h_2}^\top J_{h_1}^\top E + J_{h_2}^\top J_E h_1 + J_{J_{h_1}^\top E + J_E h_1} h_2.$$

The last two terms can be written as

$$\begin{aligned}
&J_{h_2}^\top J_E h_1 + J_{J_{h_1}^\top E + J_E h_1} h_2 \\
&\qquad\qquad = \nabla\Big(h_2^\top\big(\nabla(h_1^\top E) + \operatorname{curl} E \times h_1\big)\Big) + \operatorname{curl}\big(\operatorname{curl} E \times h_1\big) \times h_2.
\end{aligned}$$

This leads to

$$\begin{aligned}
&J_{h_2}^\top J_E h_1 + J_{J_{h_1}^\top E + J_E h_1} h_2 \\
&\qquad\qquad = \nabla\Big(h_2^\top\big(\nabla(h_1^\top E) + \operatorname{curl} E \times h_1\big)\Big) + \big(A_1 \operatorname{curl} E\big) \times h_2 \\
&\qquad\qquad\qquad\qquad + k^2(E \times h_1) \times h_2 + \nabla\big(h_1^\top \operatorname{curl} E\big) \times h_2.
\end{aligned}$$

Now we consider

$$\begin{aligned}
\mathcal{A}\big((E_1')_2', V\big) &= \mathcal{A}(W_1', V) - \mathcal{A}(J_{h_1}^\top E_2' + J_{E_2'} h_1 - J_{h_2}^\top W_1 - J_{W_1} h_2, V) \\
&= \int_\Omega \Big(\operatorname{curl} W_1^\top A_2 \overline{\operatorname{curl} V} + k^2 W_1^\top A_2 \overline{V}\Big)\,\mathrm{d}x \\
&\quad + \int_\Omega \Big(\operatorname{curl} W_2^\top A_1 \overline{\operatorname{curl} V} + k^2 W_2^\top A_1 \overline{V}\Big)\,\mathrm{d}x \\
&\quad + \int_\Omega \operatorname{curl} E^\top \Big(J_{h_2}^\top A_1 + A_1 J_{h_2} - \operatorname{div}(h_2) A_1 + A_1'(h_2)\Big)\overline{\operatorname{curl} V}\,\mathrm{d}x \\
&\quad + k^2 \int_\Omega E^\top \Big(- J_{h_2} A_1 - A_1 J_{h_2}^\top + \operatorname{div}(h_2) A_1 + A_1'(h_2)\Big)\overline{V}\,\mathrm{d}x \\
&\quad - \mathcal{A}(J_{h_1}^\top E_2' + J_{E_2'} h_1, V) - \mathcal{A}(J_{h_2}^\top E_1' + J_{E_1'} h_2, V) \\
&\quad - \mathcal{A}(J_{h_2}^\top J_{h_1}^\top E + J_{h_2}^\top J_E h_1 + J_{J_{h_1}^\top E + J_E h_1} h_2, V).
\end{aligned}$$

We use our previous calculations to get

$$\begin{aligned}
&\mathcal{A}\big((E_1')_2'), V\big) \\
&= \underbrace{\int_\Omega \Big(\operatorname{curl} E_1'^\top A_2 \overline{\operatorname{curl} V} + k^2 E_1'^\top A_2 \overline{V}\Big)\,\mathrm{d}x - \mathcal{A}(J_{h_2} E_1' + J_{E_1'} h_2, V)}_{=0} \\
&\quad + \underbrace{\int_\Omega \Big(\operatorname{curl} E_2'^\top A_1 \overline{\operatorname{curl} V} + k^2 E_2'^\top A_1 \overline{V}\Big)\,\mathrm{d}x - \mathcal{A}(J_{h_1} E_2' + J_{E_2'} h_1, V)}_{=0} \\
&\quad + \int_\Omega \Big(A_2 \operatorname{curl} E + k^2(E \times h_2) + \nabla(h_2^\top \operatorname{curl} E)\Big) A_1 \overline{\operatorname{curl} V}\,\mathrm{d}x \\
&\quad + \int_\Omega \Big(A_1 \operatorname{curl} E + k^2(E \times h_1) + \nabla(h_1^\top \operatorname{curl} E)\Big) A_2 \overline{\operatorname{curl} V}\,\mathrm{d}x
\end{aligned}$$

$$
\begin{aligned}
&+ k^2 \int_\Omega \Big(\operatorname{curl} E \times h_2 + \nabla(h_2^\top E)\Big)^\top A_1 \overline{V} \,\mathrm{d}x \\
&+ k^2 \int_\Omega \Big(\operatorname{curl} E \times h_1 + \nabla(h_1^\top E)\Big)^\top A_2 \overline{V} \,\mathrm{d}x \\
&+ \int_\Omega \operatorname{curl} E^\top \Big(J_{h_2}^\top A_1 + A_1 J_{h_2} - \operatorname{div}(h_2) A_1 + A_1'(h_2)\Big) \overline{\operatorname{curl} V} \,\mathrm{d}x \\
&+ k^2 \int_\Omega E^\top \Big(- J_{h_2} A_1 - A_1 J_{h_2}^\top + \operatorname{div}(h_2) A_1 + A_1'(h_2)\Big) \overline{V} \,\mathrm{d}x \\
&- \int_\Omega \operatorname{curl} \Big[(A_1 \operatorname{curl} E) \times h_2 + k^2 (E \times h_1) \times h_2 \\
&\qquad + \nabla(h_1^\top \operatorname{curl} E) \times h_2 \Big]^\top \overline{\operatorname{curl} V} \,\mathrm{d}x \\
&+ k^2 \int_\Omega \Big[\nabla \Big(h_2^\top \big(\nabla(h_1^\top E) + \operatorname{curl} E \times h_1\big)\Big) + (A_1 \operatorname{curl} E) \times h_2 \\
&\qquad + k^2 (E \times h_1) \times h_2 + \nabla(h_1^\top \operatorname{curl} E) \times h_2 \Big]^\top \overline{V} \,\mathrm{d}x.
\end{aligned}
$$

Recall $A_i = \operatorname{div}(h_i) I - J_{h_i} - J_{h_i}^\top$. Therefore, we have

$$
A_2 A_1 + A_1 A_2 = 2 \operatorname{div}(h_2) A_1 - J_{h_2} A_1 - J_{h_2}^\top A_1 - A_1 J_{h_2} - A_1 J_{h_2}^\top,
$$

which leads to

$$
\begin{aligned}
\mathcal{A}\big((E_1')_2', V\big) &= k^2 \int_\Omega E^\top \Big(- J_{h_2} A_1 - A_1 J_{h_2}^\top + \operatorname{div}(h_2) A_1 + A_1'(h_2)\Big) \overline{V} \,\mathrm{d}x \\
&+ \int_\Omega \operatorname{curl} E^\top \Big(- J_{h_2} A_1 - A_1 J_{h_2}^\top + \operatorname{div}(h_2) A_1 + A_1'(h_2)\Big) \overline{\operatorname{curl} V} \,\mathrm{d}x \\
&+ \int_\Omega \Big(k^2 (E \times h_2) + \nabla(h_2^\top \operatorname{curl} E)\Big) A_1 \overline{\operatorname{curl} V} \,\mathrm{d}x \\
&+ \int_\Omega \Big(k^2 (E \times h_1) + \nabla(h_1^\top \operatorname{curl} E)\Big) A_2 \overline{\operatorname{curl} V} \,\mathrm{d}x \\
&+ k^2 \int_\Omega \Big(\operatorname{curl} E \times h_2 + \nabla(h_2^\top E)\Big)^\top A_1 \overline{V} \,\mathrm{d}x \\
&+ k^2 \int_\Omega \Big(\operatorname{curl} E \times h_1 + \nabla(h_1^\top E)\Big)^\top A_2 \overline{V} \,\mathrm{d}x \\
&- \int_\Omega \operatorname{curl} \Big[(A_1 \operatorname{curl} E) \times h_2 + k^2 (E \times h_1) \times h_2 \\
&\qquad + \nabla(h_1^\top \operatorname{curl} E) \times h_2 \Big]^\top \overline{\operatorname{curl} V} \,\mathrm{d}x
\end{aligned}
$$

$$+ k^2 \int_\Omega \Big[\nabla\Big(h_2^\top\big(\nabla(h_1^\top E) + \operatorname{curl} E \times h_1\big)\Big) + (A_1 \operatorname{curl} E) \times h_2$$
$$+ k^2 (E \times h_1) \times h_2 + \nabla(h_1^\top \operatorname{curl} E) \times h_2\Big]^\top \overline{V}\, \mathrm{d}x. \tag{3.1.15}$$

For vector fields E, V, h and a symmetric matrix A we can show the following identities by using elementary calculus:

$$\begin{aligned}
\operatorname{div}\big((h^\top E)V\big) &= (h^\top E)\operatorname{div}(V) + V^\top J_h^\top E + V^\top J_E^\top h,\\
\operatorname{div}\big((h^\top V)AE\big) &= (h^\top V)\operatorname{div}(AE) + E^\top A J_h^\top V + E^\top A J_V^\top h,\\
\operatorname{div}\big((h^\top E)AV\big) &= (h^\top E)\operatorname{div}(AV) + V^\top A J_h^\top E + V^\top A J_E^\top h,\\
\operatorname{div}\big((E^\top AV)h\big) &= E^\top AV\operatorname{div}(h) + h^\top J_E^\top AV + E^\top A'(h)V + E^\top A J_V h.
\end{aligned}$$

Together with the identity $(J_F - J_F^\top)G = \operatorname{curl} F \times G$ for two vector fields F and G, we have

$$\begin{aligned}
&\operatorname{curl} E^\top\Big(- J_{h_2}A_1 - A_1 J_{h_2}^\top + \operatorname{div}(h_2)A_1 + A_1'(h_2)\Big)\overline{\operatorname{curl} V}\\
&= -\operatorname{div}\Big[(h_2^\top \operatorname{curl} E)A_1\overline{\operatorname{curl} V} + (h_2^\top\overline{\operatorname{curl} V})A_1 \operatorname{curl} E - (\operatorname{curl} E^\top A_1 \overline{\operatorname{curl} V})h_2\Big]\\
&\quad + (h_2^\top\overline{\operatorname{curl} V})\operatorname{div}(A_1 E) + (h_2^\top \operatorname{curl} E)\operatorname{div}(A_1\overline{\operatorname{curl} V})\\
&\quad + (A_1 \operatorname{curl} E)^\top(\overline{\operatorname{curl}\operatorname{curl} V} \times h_2) - k^2 (E \times h_2)^\top A_1 \overline{\operatorname{curl} V},
\end{aligned} \tag{3.1.16}$$

since $\operatorname{curl}\operatorname{curl} E = k^2 E$. Similarly, we have

$$\begin{aligned}
&E^\top\Big(- J_{h_2}A_1 - A_1 J_{h_2}^\top + \operatorname{div}(h_2)A_1 + A_1'(h_2)\Big)\overline{V}\\
&= -\operatorname{div}\Big[(h_2^\top E)A_1\overline{V} + (h_2^\top\overline{V})A_1 E + (E^\top A_1\overline{V})h_2\Big] + (h_2^\top\overline{V})\operatorname{div}(A_1 E)\\
&\quad + (h_2^\top E)\operatorname{div}(A_1\overline{V}) - (A_1 E)^\top(\overline{\operatorname{curl} V} \times h_2) - (\operatorname{curl} E \times h_2)^\top A_1\overline{V}
\end{aligned} \tag{3.1.17}$$

and

$$\operatorname{div}\Big((h_2^\top E)A_1\overline{V}\Big) = (h_2^\top E)\operatorname{div}(A_1\overline{V} + \nabla(h_2^\top E)^\top A_1\overline{V}, \tag{3.1.18}$$

$$\begin{aligned}
\operatorname{div}\Big((h_2^\top \operatorname{curl} E)A_1\overline{\operatorname{curl} V}\Big) &= (h_2^\top \operatorname{curl} E)\operatorname{div}(A_1\overline{\operatorname{curl} V})\\
&\quad + \nabla(h_2^\top \operatorname{curl} E)^\top A_1\overline{\operatorname{curl} V}.
\end{aligned} \tag{3.1.19}$$

Combining (3.1.16), (3.1.17), (3.1.18) and (3.1.19) and inserting the result into (3.1.15) yields

$$\mathcal{A}\big((E_1')_2', V\big)$$

$$
\begin{aligned}
&= \int_\Omega \operatorname{div}\left[(\operatorname{curl} E^\top A_1 \overline{\operatorname{curl} V}) h_2 - (h_2^\top \overline{\operatorname{curl} V} A_1 \operatorname{curl} E)\right] \mathrm{d}x \\
&\quad + \int_\Omega \Big((h_2^\top \overline{\operatorname{curl} V}) \operatorname{div}(A_1 \operatorname{curl} E) \\
&\qquad\qquad - (A_1 \operatorname{curl} E)^\top (\overline{\operatorname{curl}\operatorname{curl} V} \times h_2) \Big) \mathrm{d}x \\
&\quad + k^2 \int_\Omega \operatorname{div}\left[(E^\top A_1 \overline{V}) h_2 - (h_2^\top \overline{V}) A_1 E\right] \mathrm{d}x \\
&\quad + k^2 \int \Big((h_2^\top \overline{V}) \operatorname{div}(A_1 E) - (A_1 E)(\overline{\operatorname{curl} V} \times h_2) \Big) \mathrm{d}x \\
&\quad + \int_\Omega \Big(k^2 (E \times h_1) + \nabla(h_1^\top \operatorname{curl} E) \Big)^\top A_2 \overline{\operatorname{curl} V} \, \mathrm{d}x \\
&\quad + k^2 \int_\Omega \Big(\operatorname{curl} E \times h_1 + \nabla(h_1^\top E) \Big)^\top A_2 \overline{V} \, \mathrm{d}x \\
&\quad - \int_\Omega \operatorname{curl} \Big((A_1 \operatorname{curl} E) \times h_2 + k^2 (E \times h_1) \times h_2 \\
&\qquad\qquad + \nabla(h_1^\top \operatorname{curl} E) \times h_2 \Big)^\top \overline{\operatorname{curl} V} \, \mathrm{d}x \\
&\quad + k^2 \int_\Omega \Big[\nabla \Big(h_2^\top \big(\nabla(h_1^\top E) + \operatorname{curl} E \times h_1 \big) \Big) + (A_1 \operatorname{curl} E) \times h_2 \\
&\qquad\qquad + k^2 (E \times h_1) \times h_2 + \nabla(h_1^\top \operatorname{curl} E) \times h_2 \Big]^\top \overline{V} \, \mathrm{d}x.
\end{aligned}
$$

By the Theorem of Gauß, we have

$$
\begin{aligned}
&\int_\Omega \operatorname{div}\left[(\operatorname{curl} E^\top A_1 \overline{\operatorname{curl} V}) h_2 - (h_2^\top \overline{\operatorname{curl} V}) A_1 \operatorname{curl} E\right] \mathrm{d}x \\
&\qquad = - \int_{\partial D} \Big(h_{2,\nu} (\operatorname{curl} E^\top A_1 \overline{\operatorname{curl} V}) - (A_1 \operatorname{curl} E)_\nu (h_2^\top \overline{\operatorname{curl} V}) \Big) \mathrm{d}s,
\end{aligned}
$$

since h_1, h_2 are compactly supported in Ω. On the other hand, using the partial integration formula for the curl operator (2.2.2), we have

$$
\begin{aligned}
&\int_\Omega \Big(- (A_1 \operatorname{curl} E)^\top (\overline{\operatorname{curl}\operatorname{curl} V} \times h_2) - \operatorname{curl} \big((A_1 \operatorname{curl} E) \times h_2 \big)^\top \overline{\operatorname{curl} V} \Big) \\
&= \int_\Omega \Big((A_1 \operatorname{curl} E \times h_2)^\top \overline{\operatorname{curl}\operatorname{curl} V} - \operatorname{curl} \big((A_1 \operatorname{curl} E) \times h_2 \big)^\top \overline{\operatorname{curl} V} \Big) \mathrm{d}x \\
&= - \int_{\partial D} (\nu \times \overline{\operatorname{curl} V})^\top \big((A_1 \operatorname{curl} E) \times h_2 \big) \mathrm{d}s.
\end{aligned}
$$

Note that in both cases we have used the outwards directed normal vector ν to ∂D, which points inwards Ω. In the boundary integral, we only need the tangential component of $(A_1 \operatorname{curl} E) \times h_2$, which is given by

$$[(A_1 \operatorname{curl} E) \times h_2]_\tau = (A_1 \operatorname{curl} E)_\nu (\nu \times h_2) - \big(\nu \times (A_1 \operatorname{curl} E)\big) h_{2,\nu}.$$

Since the tangential trace of V vanishes on ∂D, i.e. $\nu \times \overline{V} = 0$, we have $(\operatorname{curl} \overline{V})_\nu = -\operatorname{Div}(\nu \times \overline{V}) = 0$. Therefore we have

$$\begin{aligned}(\nu \times \overline{\operatorname{curl} V})^\top &\big((A_1 \operatorname{curl} E) \times h_2\big) \\ &= (h_2^\top \overline{\operatorname{curl} V})(A_1 \operatorname{curl} E)_\nu - h_{2,\nu}(\operatorname{curl} E^\top A_1 \overline{\operatorname{curl} V}).\end{aligned}$$

We finally conclude

$$\begin{aligned}&\int_\Omega \operatorname{div} \Big[(\operatorname{curl} E^\top A_1 \overline{\operatorname{curl} V}) h_2 - (h_2^\top \overline{\operatorname{curl} V}) A_1 \operatorname{curl} E\Big] \, \mathrm{d}x \\ -&\int_\Omega \Big((A_1 \operatorname{curl} E)^\top (\overline{\operatorname{curl} \operatorname{curl} V} \times h_2) - \operatorname{curl}\big((A_1 \operatorname{curl} E) \times h_2\big)^\top \overline{\operatorname{curl} V}\Big) \, \mathrm{d}x = 0.\end{aligned}$$

A second application of the Theorem of Gauß leads together with $\nu \times E = \nu \times \overline{V} = 0$, i.e $E = E_\nu \nu$, $\overline{V} = \overline{V}_\nu \nu$ on ∂D to

$$\begin{aligned}&\int_\Omega \operatorname{div} \Big[(E^\top A_1 \overline{V}) h_2 - (h_2^\top \overline{V}) A_1 E\Big] \, \mathrm{d}x \\ &\qquad = -\int_{\partial D} \Big((\nu^\top A_1 \nu) h_{2,\nu} E_\nu \overline{V}_\nu - (\nu^\top A_1 \nu) h_{2,\nu} E_\nu \overline{V}_\nu\Big) \, \mathrm{d}s = 0.\end{aligned}$$

We have achieved

$$\begin{aligned}\mathcal{A}\big((E_1')_2', V\big) = &\int_\Omega \Big((h_2^\top \overline{\operatorname{curl} V}) \operatorname{div}(A_1 \operatorname{curl} E) + k^2 (h_2^\top \overline{V}) \operatorname{div}(A_1 E)\Big) \, \mathrm{d}x \\ &- k^2 \int_\Omega \Big((A_1 E)^\top (\overline{\operatorname{curl} V} \times h_2)\Big) \, \mathrm{d}x \\ &+ k^2 \int_\Omega \Big(\operatorname{curl} E \times h_1 + \nabla(h_1^\top E)\Big)^\top A_2 \overline{V} \, \mathrm{d}x \\ &+ \int_\Omega \Big(k^2 (E \times h_1) + \nabla(h_1^\top \operatorname{curl} E)\Big)^\top A_2 \overline{\operatorname{curl} V} \, \mathrm{d}x \\ &- \int_\Omega \operatorname{curl} \Big(k^2 (E \times h_1) \times h_2 + \nabla(h_1^\top \operatorname{curl} E) \times h_2\Big)^\top \overline{\operatorname{curl} V} \, \mathrm{d}x \\ &+ k^2 \int_\Omega \Big[\nabla\Big(h_2^\top \big(\nabla(h_1^\top E) + \operatorname{curl} E \times h_1\big)\Big) + (A_1 \operatorname{curl} E) \times h_2\end{aligned}$$

$$+ k^2(E \times h_1) \times h_2 + \nabla(h_1^\top \operatorname{curl} E) \times h_2\Big]^\top \overline{V}\,\mathrm{d}x.$$

We take a closer look at the term $\operatorname{curl}\big((E \times h_1) \times h_2\big)$. Similar calculations as before lead to

$$\begin{aligned}
&\operatorname{curl}\big((E \times h_1) \times h_2\big)\\
=&A_2(E \times h_1) - h_2 \operatorname{div}(E \times h_1) + \nabla\big(h_2^\top (E \times h_1)\big) + \operatorname{curl}(E \times h_1) \times h_2\\
=&A_2(E \times h_1) - h_2 \operatorname{div}(E \times h_1) + \nabla\big(h_2^\top (E \times h_1)\big)\\
&\quad + (A_1 E) \times h_2 + \big(\nabla(h_1^\top E)\big) \times h_2 + (\operatorname{curl} E \times h_1) \times h_2.
\end{aligned}$$

This leads to

$$\begin{aligned}
\mathcal{A}\big((E_1')_2', V\big) = &\int_\Omega \Big((h_2^\top \overline{\operatorname{curl} V}) \operatorname{div}(A_1 \operatorname{curl} E) + k^2 (h_2^\top \overline{V}) \operatorname{div}(A_1 E)\Big)\,\mathrm{d}x\\
&+ \int_\Omega \Big(\nabla(h_1^\top \operatorname{curl} E) + k^2 \operatorname{curl} E \times h_1 + k^2 \nabla(h_1^\top E)\Big)^\top A_2 \overline{V}\,\mathrm{d}x\\
&- \int_\Omega \operatorname{curl}\Big(\nabla(h_1^\top \operatorname{curl} E) \times h_2\Big)^\top \overline{\operatorname{curl} V}\,\mathrm{d}x\\
&+ k^2 \int_\Omega \Big[\operatorname{div}(E \times h_1) h_2 - \nabla\big(h_2^\top (E \times h_1)\big)\\
&\qquad - \nabla(h_1^\top E) \times h_2 - (\operatorname{curl} E \times h_1) \times h_2\Big]^\top \overline{\operatorname{curl} V}\,\mathrm{d}x\\
&+ k^2 \int_\Omega \Big[\nabla\Big(h_2^\top \big(\nabla(h_1^\top E) + \operatorname{curl} E \times h_1\big)\Big) + (A_1 \operatorname{curl} E) \times h_2\\
&\qquad + k^2 (E \times h_1) \times h_2 + \nabla(h_1^\top \operatorname{curl} E) \times h_2\Big]^\top \overline{V}\,\mathrm{d}x.
\end{aligned}$$

Again with the Theorem of Gauß, we have

$$\begin{aligned}
&\int_\Omega \nabla\big(h_2^\top (E \times h_1)\big)^\top \overline{\operatorname{curl} V}\,\mathrm{d}x = -\int_\Omega \operatorname{div}\Big[\nabla\big(h_2^\top (E \times h_1)\big) \times \overline{V}\Big]\,\mathrm{d}x\\
=&\int_{\partial D} \nu^\top \Big(\nabla\big(h_2^\top (E \times h_1)\big) \times \overline{V}\Big)\,\mathrm{d}s = \int_{\partial D} \nabla\big(h_2^\top (E \times h_1)\big)^\top (\nu \times \overline{V})\,\mathrm{d}s = 0.
\end{aligned}$$

and similarly

$$\int_\Omega \nabla\big(h_2^\top \nabla(h_1^\top \operatorname{curl} E)\big)^\top \overline{\operatorname{curl} V}\,\mathrm{d}x = 0.$$

The last term occurs by considering

$$\operatorname{curl}\big(\nabla(h_1^\top \operatorname{curl} E) \times h_2\big)$$

$$= A_2\nabla(h_1^\top \operatorname{curl} E) - h_2\Delta(h_1^\top \operatorname{curl} E) + \nabla\big(h_2^\top\nabla(h_1^\top \operatorname{curl} E)\big).$$

This leads to

$$\begin{aligned}
\mathcal{A}\big((E_1')_2', V\big) &= \int_\Omega (h_2^\top \overline{\operatorname{curl} V})\big(\operatorname{div}(A_1 \operatorname{curl} E) + \Delta(h_1^\top \operatorname{curl} E)\big)\,\mathrm{d}x \\
&+ k^2 \int_\Omega (h_2^\top \overline{V})\big(\operatorname{div}(A_1 E) + \Delta(h_1^\top E)\big)\,\mathrm{d}x + k^2 \int_\Omega \big(\operatorname{curl} E \times h_1\big)^\top A_2 \overline{V}\,\mathrm{d}x \\
&+ k^2 \int_\Omega \Big[\nabla\big(h_2^\top(\operatorname{curl} E \times h_1)\big) + (A_1 \operatorname{curl} E) \times h_2 \\
&\qquad + k^2 (E \times h_1) \times h_2 + \nabla(h_1^\top \operatorname{curl} E) \times h_2\Big]^\top \overline{V}\,\mathrm{d}x \\
&+ k^2 \int_\Omega \Big(\operatorname{div}(E \times h_1) h_2 - (\operatorname{curl} E \times h_1) \times h_2\Big)^\top \overline{\operatorname{curl} V}\,\mathrm{d}x.
\end{aligned}$$

We apply again the partial integration formula (2.2.2) in the following way

$$\int_\Omega \big((\operatorname{curl} E \times h_1) \times h_2\big)^\top \overline{\operatorname{curl} V}\,\mathrm{d}x = \int_\Omega \big((\operatorname{curl} E \times h_1) \times h_2\big)^\top \overline{V}\,\mathrm{d}x.$$

The term on the right hand side can be calculated by

$$\begin{aligned}
&\operatorname{curl}\big((\operatorname{curl} E \times h_1) \times h_2\big) \\
=& A_2(\operatorname{curl} E \times h_1) - \operatorname{div}(\operatorname{curl} E \times h_1) h_2 + (A_1 \operatorname{curl} E) \times h_2 \\
&\quad + k^2 (E \times h_1) \times h_2 + \nabla(h_1^\top \operatorname{curl} E) \times h_2 + \nabla\big(h_2^\top(\operatorname{curl} E \times h_1)\big),
\end{aligned}$$

which leads to

$$\begin{aligned}
\mathcal{A}\big((E_1')_2', V\big) &= k^2 \int_\Omega (h_2^\top \overline{V})\Big(\operatorname{div}(A_1 E) + \Delta(h_1^\top E) + \operatorname{div}(\operatorname{curl} E \times h_1)\Big)\,\mathrm{d}x \\
&+ \int_\Omega (h_1^\top \overline{\operatorname{curl} V})\Big(\operatorname{div}(A_1 \operatorname{curl} E) + \Delta(h_1^\top \operatorname{curl} E) + k^2 \operatorname{div}(E \times h_1)\Big)\,\mathrm{d}x.
\end{aligned}$$

Since $\operatorname{div} E = 0$ and $\operatorname{curl}\operatorname{curl} E = k^2 E$ we have with some basic vector calculus the identities

$$\begin{aligned}
0 &= \operatorname{div}\big(\operatorname{curl}(E \times h_1)\big) = \operatorname{div}(A_1 E) + \Delta(h_1^\top E) + \operatorname{div}(\operatorname{curl} E \times h_1), \\
0 &= \operatorname{div}\big(\operatorname{curl}(\operatorname{curl} E \times h_1)\big) = \operatorname{div}(A_1 \operatorname{curl} E)\Delta(h_1^\top \operatorname{curl} E) + k^2 \operatorname{div}(E \times h_1).
\end{aligned}$$

With these identities, we finally conclude

$$\mathcal{A}\big((E_1')_2', V\big) = \mathcal{A}(W_1' - J_{h_1}^\top E_2' - J_{E_2'} h_1 + J_{h_2}^\top W_1 + J_{W_1} h_2, V) = 0$$

for all $V \in H_{\mathrm{pc}}(\Omega)$, i.e. $(E_1')_2'$ is a radiating solution to Maxwell's equations. $\square$

The domain derivative $(E_1')_2' \in H(\mathrm{curl}, \Omega)$ with respect to the perturbation h_2 of the material derivative E_1' with respect to the perturbation h_1 is, as a solution to the scattering problem, fully determined by its trace $\nu \times (E_1')_2'$ on ∂D. Since $W_1 \in H_{\mathrm{pc}}(\Omega)$, we have

$$\nu \times (E_1')_2' = \nu \times \Big[- J_{h_1}^\top E_2' - J_{E_2'} h_1 - J_{h_2}^\top W_1 - J_{W_1} h_2 \Big].$$

With these boundary values, we can calculate the boundary values of the second domain derivative. Our goal is to find a characterization, which shows the symmetry of the second domain derivative with respect to the perturbations h_1 and h_2. In order to formulate the characterization, we need to define the *curvature operator* $\mathcal{R}$ and the *(mean) curvature* κ. For more details, see [40, Section 2.5.6]. Let Γ be a smooth surface of a bounded and simply connected domain Ω. Then there is an open neighborhood U of Γ, such that for every $x \in U$ there is exactly one $\hat{x} \in \Gamma$ which satisfies

$$|\hat{x} - x| = \min_{u \in \Gamma} |u - x|.$$

This allows us to extend $\nu : \Gamma \to \mathbb{S}^2$ to U by setting $\nu(x) = \nu(\hat{x})$. Note that $\nu(x) = \nu(x + s\nu)$ for $x \in \Gamma$ and s sufficiently small. Furthermore, we have for any $x \in U$ with $x \notin \Gamma$

$$\nu(x) = \pm \nabla |x - \hat{x}|,$$

where the sign depends on whether x lies in Ω or in $\mathbb{R}^3 \setminus \overline{\Omega}$. This implies $\mathrm{curl}\, \nu = 0$. Now, we can define the *curvature operator* $\mathcal{R} : \Gamma \to \mathbb{R}^{3\times 3}$ by $\mathcal{R}(x) = J_\nu(x)$, $x \in \Gamma$. We state the most important properties in the following lemma.

Lemma 3.11. *Let Γ be a smooth surface. The curvature operator $\mathcal{R}$ is symmetric and is acting only on the tangential plane, i.e.*

$$\mathcal{R}(x)\nu(x) = 0, \quad x \in \Gamma.$$

Proof. Let $v \in \mathbb{R}^3$. Then symmetry of $\mathcal{R}$ follows from

$$\mathcal{R}h = J_\nu h = (J_\nu - J_\nu^\top)h + J_\nu^\top h = \underbrace{\mathrm{curl}\, \nu}_{=0} \times h + J_\nu^\top h = \mathcal{R}^\top h.$$

For $x \in \Gamma$, we have

$$1 = |\nu(x)|$$

and therefore

$$0 = \nabla(|\nu(x)|^2) = \nabla(\nu(x) \cdot \nu(x)) = 2\, J_\nu^\top(x)\nu(x) = 2\, \mathcal{R}(x)\nu(x),$$

since $\mathcal{R}$ is symmetric. $\square$

We define the *mean curvature* $\kappa : \Gamma \to \mathbb{R}$ by

$$\kappa = \frac{1}{2}\operatorname{div}(\nu). \tag{3.1.20}$$

Note that the definition of the mean curvature in [20, 23, 24] has a different sign. We have chosen the plus sign to be consistent with [25, 27, 40].

Theorem 3.12. *Let ∂D be regular. The second domain derivative E'' is a radiating solution to Maxwell's equations, satisfying the boundary condition*

$$\begin{aligned}
\nu \times E'' = &- \nu \times \Big[\operatorname{Grad}\big(h_1^\top E_2' + h_2^\top E_1'\big) + \operatorname{curl} E_2' \times h_1 + \operatorname{curl} E_1' \times h_2\Big] \\
&- \mathrm{i}k\big(h_{2,\tau}^\top \mathcal{R} h_{1,\tau}\big) H_\tau + \overrightarrow{\operatorname{Curl}}_{\partial D}\Big[\big(h_{2,\tau}^\top \mathcal{R} h_{1,\tau}\big) E_\nu + h_{1,\nu} h_{2,\nu} \frac{\partial E_\nu}{\partial \nu}\Big] \\
&+ \mathrm{i}k\, h_{1,\nu} h_{2,\nu}\Big(\mathcal{R} - 2\kappa - \frac{\partial}{\partial \nu}\Big) H_\tau \\
&+ h_{1,\nu} \overrightarrow{\operatorname{Curl}}_{\partial D}\Big[h_{2,\tau}^\top \frac{\partial E_\tau}{\partial \nu}\Big] + h_{2,\nu} \overrightarrow{\operatorname{Curl}}_{\partial D}\Big[h_{1,\tau}^\top \frac{\partial E_\tau}{\partial \nu}\Big] \\
&+ \Big(h_{1,\tau}^\top \operatorname{Grad}_{\partial D} E_\nu\Big) \overrightarrow{\operatorname{Curl}}_{\partial D} h_{2,\nu} + \Big(h_{2,\tau}^\top \operatorname{Grad}_{\partial D} E_\nu\Big) \overrightarrow{\operatorname{Curl}}_{\partial D} h_{1,\nu}
\end{aligned}$$

on ∂D.

Proof. Recall the characterization of the trace of the second domain derivative (3.1.11), which reads as

$$\nu \times E'' = \nu \times (E_1')_2' - \nu \times E_h',$$

where $h = J_{h_1} h_2$. From Theorem 3.6, we know

$$\nu \times E_h' = \overrightarrow{\operatorname{Curl}}_{\partial D}\Big(\big(\nu^\top J_{h_1} h_2\big) E_\nu\Big) - \mathrm{i}k\big(\nu^\top J_{h_1} h_2\big) H_\tau.$$

It is

$$\begin{aligned}
\nu^\top J_{h_1} h_2 &= (\nu^\top J_{h_1} \nu) h_{2,\nu} + \nu^\top J_{h_1} h_{2,\tau} \\
&= h_{2,\nu}\, \nu^\top \big(\nabla h_{1,\nu} - J_\nu^\top h_1\big) + h_{2,\tau}^\top \big(J_{h_1}^\top \nu + J_\nu^\top h_1 - J_n u^\top h_1\big) \\
&= h_{2,\nu} \frac{\partial h_{1,\nu}}{\partial \nu} - h_{2,\nu} h_1^\top \underbrace{J_\nu \nu}_{=\mathcal{R}\nu = 0} + h_{2\tau}^\top \operatorname{Grad}_{\partial D} h_{1,\nu} - h_{2,\tau}^\top \mathcal{R} h_{1,\tau}.
\end{aligned}$$

We have therefore

$$\nu \times E_h' = -\mathrm{i}k\big(h_{2,\nu} \frac{\partial h_{1,\nu}}{\partial \nu} + h_{2,\tau}^\top \operatorname{Grad}_{\partial D} h_{1,\nu}\big) H_\tau + \mathrm{i}k\big(h_{2,\tau} \mathcal{R} h_{1,\tau}\big) H_\tau$$

$$+\overrightarrow{\mathrm{Curl}}_{\partial D}\Big[E_\nu\big(h_{2,\nu}\frac{\partial h_{1,\nu}}{\partial\nu}+h_{2,\tau}^\top\,\mathrm{Grad}_{\partial D}\,h_{1,\nu}\big)\Big]-\overrightarrow{\mathrm{Curl}}_{\partial D}\Big[\big(h_{2,\tau}\mathcal{R}h_{1,\tau}\big)E_\nu\Big].$$

As seen before, we have

$$\nu\times(E_1')_2'=\nu\times\Big[-J_{h_1}^\top E_2'-J_{E_2'}h_1-J_{h_2}^\top W_1-J_{W_1}h_2\Big].$$

We use $W_i=E_i'+J_{h_i}^\top E+J_Eh_i$ for $i=1,2$ to find

$$\begin{aligned}\nu\times(E_1')_2'=&-\nu\times\Big[\mathrm{Grad}_{\partial D}\left(h_1^\top E_2'+h_2^\top E_1'\right)+\mathrm{curl}\,E_2'\times h_1+\mathrm{curl}\,E_1'\times h_2\Big]\\&-\nu\times\Big[\mathrm{Grad}_{\partial D}\Big(h_2^\top\big(\nabla(h_1^\top E)+\mathrm{curl}\,E\times h_1\big)\Big)+\mathrm{curl}(\mathrm{curl}\,E\times h_1)\times h_2\Big].\end{aligned}$$

We have identified some terms, which are not symmetric in h_1 and h_2. We take a closer look at these. We have, as seen before,

$$\mathrm{curl}(\mathrm{curl}\,E\times h_1)\times h_2=(A_1\,\mathrm{curl}\,E)\times h_2+k^2(E\times h_1)\times h_2+\nabla(h_1^\top\,\mathrm{curl}\,E)\times h_2.$$

Since $\nu\times E=0$ on ∂D, we have

$$\begin{aligned}-\nu\times\mathrm{Grad}_{\partial D}\left(h_2^\top\nabla(h_1^\top E)\right)&=\overrightarrow{\mathrm{Curl}}_{\partial D}\Big(h_{2,\tau}^\top\,\mathrm{Grad}_{\partial D}(h_1^\top E)+h_{2,\nu}\frac{\partial h_1^\top E}{\partial\nu}\Big)\\&=\mathrm{Grad}_{\partial D}\Big(h_{2,\tau}^\top\,\mathrm{Grad}_{\partial D}(h_{1,\nu}E_\nu)+h_{2,\nu}\frac{\partial(h_{1,\nu}E_\nu+h_{1,\tau}^\top E_\tau)}{\partial\nu}\Big)\end{aligned}$$

and therefore

$$\begin{aligned}-\nu\times\mathrm{Grad}_{\partial D}\left(h_2^\top\nabla(h_1^\top E)\right)=&\overrightarrow{\mathrm{Curl}}_{\partial D}\Big(E_\nu h_{2,\tau}^\top\,\mathrm{Grad}_{\partial D}\,h_{1,\nu}\\&+h_{1,\nu}h_{2,\tau}^\top\,\mathrm{Grad}_{\partial D}\,E_\nu+h_{1,\nu}\,h_{2,\nu}\frac{\partial E_\nu}{\partial\nu}+h_{2,\nu}\,E_\nu\frac{\partial h_{1,\nu}}{\partial\nu}+h_{2,\nu}h_{1,\tau}^\top\frac{\partial E_\tau}{\partial\nu}\Big).\end{aligned}$$

Next, we consider

$$\nu\times\big((E\times h_1)\times h_2\big)=E_\nu\,h_{2,\nu}(\nu\times h_1)$$

as well as

$$\nu\times\big(\mathrm{Grad}_{\partial D}(h_1^\top\,\mathrm{curl}\,E)\times h_2\big)=\mathrm{i}k\,h_{2,\nu}\,\mathrm{Grad}_{\partial D}(h_{1,\tau}^\top H_\tau)-\mathrm{i}k\,\frac{\partial h_{1,\tau}^\top H_\tau}{\partial\nu}h_{2,\tau}$$

and since $0=(\mathrm{curl}\,E)_\nu$, i.e. $\mathrm{curl}\,E=\mathrm{i}k\,H_\tau$ we have

$$\nu\times\big((A_1\,\mathrm{curl}\,E)\times h_2\big)=\mathrm{i}k\,h_{2,\nu}A_1H_\tau-\mathrm{i}k(\nu^\top A_1H_\tau)h_{2,\tau}$$

and finally

$$\nu \times \operatorname{Grad}_{\partial D}\left(h_2^\top(\operatorname{curl} E \times h_1)\right) \\ = \overrightarrow{\operatorname{Curl}}_{\partial D}\Big(h_{2,\nu} \operatorname{curl} E^\top(\nu \times h_1) - h_{1,\nu}(\nu \times h_2)^\top \operatorname{curl} E\Big).$$

We plug these identities into (3.1.11) to get

$$\begin{aligned}\nu \times E'' = {} & \overrightarrow{\operatorname{Curl}}_{\partial D}\big(h_1^\top E_2' + h_2^\top E_1'\big) - \nu \times \Big(\operatorname{curl} E_2' \times h_1 + \operatorname{curl} E_1' \times h_2\Big) \\ & - \mathrm{i}k\big(h_{2,\tau}^\top \mathcal{R} h_{1,\tau}\big) H_\tau + \overrightarrow{\operatorname{Curl}}_{\partial D}\Big[\big(h_{2,\tau}^\top \mathcal{R} h_{1,\tau}\big) E_\nu + h_{1,\nu}\, h_{2,\nu} \frac{\partial E_\nu}{\partial \nu}\Big] \\ & + \overrightarrow{\operatorname{Curl}}_{\partial D}\Big[h_{1,\nu}\, h_{2,\tau}^\top \operatorname{Grad} E_\nu + h_{2,\nu}\, h_{1,\tau}^\top \frac{\partial E_\tau}{\partial \nu}\Big] \\ & - \overrightarrow{\operatorname{Curl}}_{\partial D}\Big[h_{2,\nu} \operatorname{curl} E^\top(\nu \times h_1) - h_{1,\nu}(\nu \times h_2)^\top \operatorname{curl} E\Big] \\ & - \mathrm{i}k\big(h_{2,\nu}\, A_1 H_\tau - (\nu^\top A_1 H_\tau) h_{2,\tau}\big) - k^2 E_\nu\, h_{2,\nu}(\nu \times h_1) \\ & - \mathrm{i}k h_{2,\nu} \operatorname{Grad}_{\partial D}(h_{1,\tau} H_\tau) \\ & + \mathrm{i}k h_{2,\tau} \frac{\partial h_{1,\tau}^\top H_\tau}{\partial \nu} + \mathrm{i}k\Big(h_{2,\nu} \frac{\partial h_{1,\nu}}{\partial \nu} + h_{2,\tau}^\top \operatorname{Grad}_{\partial D} h_{1,\nu}\Big) H_\tau.\end{aligned}$$

Note, that the first two lines are already as stated in the theorem. For any vector field F, we have

$$\frac{\partial F_\tau}{\partial \nu} = \operatorname{curl} F \times \nu + \operatorname{Grad}_{\partial D} F_\nu - \mathcal{R} F_\tau,$$

see equation (5.4.50) in [40]. Recall $A_1 = \operatorname{div}(h_1) I - J_{h_1} - J_{h_1}^\top$. Therefore, we have

$$\nu^\top A_1 H_\tau = -H_\tau^\top\big(J_{h_1} + J_{h_1}^\top\big)\nu = -H_\tau^\top \operatorname{Grad}_{\partial D} h_{1,\nu} - H_\tau^\top \mathcal{R} h_{1,\tau} - H_\tau^\top \frac{\partial h_1}{\partial \nu}.$$

We have

$$\frac{\partial h_1}{\partial \nu} - \frac{\partial h_{1,\tau}}{\partial \nu} = \frac{\partial h_{1,\nu} \nu}{\partial \nu} = h_{1,\nu} \underbrace{\frac{\partial \nu}{\partial \nu}}_{=\mathcal{R}\nu = 0} + \nu \frac{\partial h_{1,\nu}}{\partial \nu},$$

and therefore

$$(\nu^\top A_1 H_\tau) + \frac{\partial h_{1,\tau}^\top H_\tau}{\partial \nu} = -H_\tau^\top \operatorname{Grad}_{\partial D} h_{1,\nu}.$$

Additionally, using $\operatorname{div}(H) = 0$ and $H_\nu = 0$, we have

$$A_1 H\big|_\tau = \operatorname{curl}(H \times h_1)\big|_\tau - \operatorname{Grad}_{\partial D}(h_{1,\tau}^\top H_\tau) - \mathrm{i}k\, E_\nu(\nu \times h_1).$$

This leads to

$$\begin{aligned}\nu \times E'' &= \overrightarrow{\mathrm{Curl}}_{\partial D}\big(h_1^\top E_2' + h_2^\top E_1'\big) - \nu \times \Big(\operatorname{curl} E_2' \times h_1 + \operatorname{curl} E_1' \times h_2\Big)\\
&\quad - \mathrm{i}k\big(h_{2,\tau}^\top \mathcal{R} h_{1,\tau}\big) H_\tau + \overrightarrow{\mathrm{Curl}}_{\partial D}\Big[\big(h_{2,\tau}^\top \mathcal{R} h_{1,\tau}\big) E_\nu + h_{1,\nu}\, h_{2,\nu} \frac{\partial E_\nu}{\partial \nu}\Big]\\
&\quad + \overrightarrow{\mathrm{Curl}}_{\partial D}\Big[h_{1,\nu}\, h_{2,\tau}^\top \operatorname{Grad}_{\partial D} E_\nu + h_{2,\nu}\, h_{1,\tau}^\top \frac{\partial E_\tau}{\partial \nu}\Big]\\
&\quad - \overrightarrow{\mathrm{Curl}}_{\partial D}\Big[h_{2,\nu} \operatorname{curl} E^\top (\nu \times h_1) - h_{1,\nu} (\nu \times h_2)^\top \operatorname{curl} E\Big]\\
&\quad - \mathrm{i}k\, h_{2,\nu} \operatorname{curl}(H \times h_1)\\
&\quad + \mathrm{i}k\Big(h_{2,\nu} \frac{\partial h_{1,\nu}}{\partial \nu} H_\tau + \operatorname{Grad}_{\partial D}(h_{1,\nu}) \times (H_\tau \times h_{2,\tau})\Big).\end{aligned}$$

For a vector field F, the tangential part of the curl operator is given by

$$\operatorname{curl} F\big|_\tau = \overrightarrow{\mathrm{Curl}}_{\partial D} F_\nu + \Big(\mathcal{R} - 2\kappa - \frac{\partial}{\partial \nu}\Big)(F \times \nu),$$

see [40, Theorem 2.5.20]. We want to apply this identity for $F = H \times h_1$. It is $(H \times h_1) \times \nu = H_\nu h_1 - h_{1,\nu} H_\tau = -h_{1,\nu} H_\tau$ and $(H \times h_1)_\nu = \frac{1}{\mathrm{i}k} \operatorname{curl} E^\top (h_1 \times \nu)$. Therefore, we have

$$\begin{aligned}\mathrm{i}k h_{2,\nu} \operatorname{curl}(H \times h_1)\big|_\tau &= h_{2,\nu} \overrightarrow{\mathrm{Curl}}_{\partial D}\big(\operatorname{curl} E^\top (h_1 \times \nu)\big)\\
&\quad - \mathrm{i}k h_{1,\nu}\, h_{2,\nu} \big(\mathcal{R} - 2\kappa\big) H_\tau + \mathrm{i}k h_{1,\nu} h_{2,\nu} \frac{\partial H_\tau}{\partial \nu} + \mathrm{i}k h_{2,\nu} \frac{\partial h_{1,\nu}}{\partial \nu} H_\tau.\end{aligned}$$

We arrive at

$$\begin{aligned}\nu \times E'' &= \overrightarrow{\mathrm{Curl}}_{\partial D}\big(h_1^\top E_2' + h_2^\top E_1'\big) - \nu \times \Big(\operatorname{curl} E_2' \times h_1 + \operatorname{curl} E_1' \times h_2\Big)\\
&\quad - \mathrm{i}k\big(h_{2,\tau}^\top \mathcal{R} h_{1,\tau}\big) H_\tau + \overrightarrow{\mathrm{Curl}}_{\partial D}\Big[\big(h_{2,\tau}^\top \mathcal{R} h_{1,\tau}\big) E_\nu + h_{1,\nu}\, h_{2,\nu} \frac{\partial E_\nu}{\partial \nu}\Big]\\
&\quad + \mathrm{i}k h_{1,\nu}\, h_{2,\nu} \Big(\mathcal{R} - 2\kappa - \frac{\partial}{\partial \nu}\Big) H_\tau\\
&\quad + \overrightarrow{\mathrm{Curl}}_{\partial D}\Big[h_{1,\nu}\, h_{2,\tau}^\top \operatorname{Grad}_{\partial D} E_\nu + h_{2,\nu}\, h_{1,\tau}^\top \frac{\partial E_\tau}{\partial \nu}\Big]\\
&\quad - \overrightarrow{\mathrm{Curl}}_{\partial D}\Big[h_{2,\nu} \operatorname{curl} E^\top (\nu \times h_1) - h_{1,\nu} (\nu \times h_2)^\top \operatorname{curl} E\Big]\\
&\quad - h_{2,\nu} \overrightarrow{\mathrm{Curl}}_{\partial D}\big(\operatorname{curl} E^\top (h_1 \times \nu)\big)\\
&\quad + \mathrm{i}k\Big(\operatorname{Grad}_{\partial D}(h_{1,\nu}) \times (H_\tau \times h_{2,\tau})\Big).\end{aligned}$$

Since $E_\tau = \nu \times (E \times \nu) = 0$ on ∂D, we have

$$\begin{aligned}
\nu \times E'' = {} & \overrightarrow{\mathrm{Curl}}_{\partial D}\big(h_1^\top E_2' + h_2^\top E_1'\big) - \nu \times \Big(\operatorname{curl} E_2' \times h_1 + \operatorname{curl} E_1' \times h_2\Big) \\
& - \mathrm{i}k\big(h_{2,\tau}^\top \mathcal{R} h_{1,\tau}\big) H_\tau + \overrightarrow{\mathrm{Curl}}_{\partial D}\Big[\big(h_{2,\tau}^\top \mathcal{R} h_{1,\tau}\big) E_\nu + h_{1,\nu}\, h_{2,\nu} \frac{\partial E_\nu}{\partial \nu}\Big] \\
& + \mathrm{i}k h_{1,\nu}\, h_{2,\nu}\Big(\mathcal{R} - 2\kappa - \frac{\partial}{\partial \nu}\Big) H_\tau \\
& + \overrightarrow{\mathrm{Curl}}_{\partial D}\Big[h_{1,\nu}\, h_{2,\tau}^\top \frac{\partial E_\tau}{\partial \nu} + h_{2,\nu}\, h_{1,\tau}^\top \frac{\partial E_\tau}{\partial \nu}\Big] \\
& - \overrightarrow{\mathrm{Curl}}_{\partial D}\Big[h_{2,\nu} \operatorname{curl} E^\top (\nu \times h_1) - h_{1,\nu} (\nu \times h_2)^\top \operatorname{curl} E\Big] \\
& - \operatorname{curl} E^\top (\nu \times h_1) \overrightarrow{\mathrm{Curl}}_{\partial D}(h_{2,\nu}) \\
& + \mathrm{i}k\Big(\operatorname{Grad}_{\partial D}(h_{1,\nu}) \times (H_\tau \times h_{2,\tau})\Big).
\end{aligned}$$

With

$$\mathrm{i}k \operatorname{Grad}_{\partial D}(h_{1,\nu}) \times (H_\tau \times h_{2,\tau}) = -\operatorname{curl} E^\top (\nu \times h_2) \overrightarrow{\mathrm{Curl}}_{\partial D}(h_{1,\nu}),$$

we finally arrive at a symmetric characterization, i.e.

$$\begin{aligned}
\nu \times E'' = {} & \overrightarrow{\mathrm{Curl}}_{\partial D}\big(h_1^\top E_2' + h_2^\top E_1'\big) - \nu \times \Big(\operatorname{curl} E_2' \times h_1 + \operatorname{curl} E_1' \times h_2\Big) \\
& - \mathrm{i}k\big(h_{2,\tau}^\top \mathcal{R} h_{1,\tau}\big) H_\tau + \overrightarrow{\mathrm{Curl}}_{\partial D}\Big[\big(h_{2,\tau}^\top \mathcal{R} h_{1,\tau}\big) E_\nu + h_{1,\nu}\, h_{2,\nu} \frac{\partial E_\nu}{\partial \nu}\Big] \\
& + \mathrm{i}k h_{1,\nu}\, h_{2,\nu}\Big(\mathcal{R} - 2\kappa - \frac{\partial}{\partial \nu}\Big) H_\tau \\
& + \overrightarrow{\mathrm{Curl}}_{\partial D}\Big[h_{1,\nu}\, h_{2,\tau}^\top \frac{\partial E_\tau}{\partial \nu} + h_{2,\nu}\, h_{1,\tau}^\top \frac{\partial E_\tau}{\partial \nu}\Big] \\
& - \overrightarrow{\mathrm{Curl}}_{\partial D}\Big[h_{2,\nu} \operatorname{curl} E^\top (\nu \times h_1) - h_{1,\nu} (\nu \times h_2)^\top \operatorname{curl} E\Big] \\
& - \operatorname{curl} E^\top (\nu \times h_1) \overrightarrow{\mathrm{Curl}}_{\partial D}(h_{2,\nu}) - \operatorname{curl} E^\top (\nu \times h_2) \overrightarrow{\mathrm{Curl}}_{\partial D}(h_{1,\nu}).
\end{aligned}$$

Considering again only the tangential part of $\operatorname{curl} E$ and using $\nu \times E = 0$, we arrive at the in the theorem stated equation. □

We do not claim this characterization to be the most elegant or the shortest characterization of E''. Our goal was to present a characterization of the second domain derivative as a scattering problem with inhomogeneous boundary condition, where the boundary condition depends on the solution (E, H) and is symmetric with respect to the perturbations h_1 and h_2.

3.2. Penetrable obstacles

The existence and characterization of the domain derivative for the scattering from penetrable obstacles using the weak formulation Ansatz has been shown in [26]. For completeness and since we will use the domain derivative in Section 4 and talk about numerical implementation in Section 6.3, we present the final result. The differences in the formulation are due to a different rescaling of Maxwell's equations. To keep the formulas short, we further assume $\sigma_D = 0$. Since we have to consider traces on ∂D from inside and outside of D, we denote with γ_T^+, γ_t^+ the traces defined on $H(\mathrm{curl}, B_R(0) \setminus \overline{D})$ and with γ_T^-, γ_t^- the traces defined on $H(\mathrm{curl}, D)$.

Theorem 3.13. *Let ∂D be of class C^1. The domain derivative (E', H') of the scattering problem (2.1.5a) - (2.1.5e) is given by the radiating weak solution of*

$$\mathrm{curl}\, E' = \mathrm{i}\kappa\, H', \quad \mathrm{curl}\, H' = -\mathrm{i}\kappa\, E' \quad \text{in } D, \tag{3.2.1}$$

$$\mathrm{curl}\, E' = \mathrm{i}k\, H', \quad \mathrm{curl}\, H' = -\mathrm{i}k\, E' \quad \text{in } \mathbb{R}^3 \setminus \overline{D}, \tag{3.2.2}$$

with transmission conditions

$$\begin{aligned} \frac{1}{\sqrt{\varepsilon_0}} \nu \times E'\big|_+ - \frac{1}{\sqrt{\varepsilon_D}} \nu \times E'\big|_- &= \frac{1}{\sqrt{\varepsilon_0}} \left(\overrightarrow{\mathrm{Curl}}_{\partial D}(h_\nu E_\nu\big|_+) - \mathrm{i}k h_\nu \gamma_T^+ H \right) \\ &\quad - \frac{1}{\sqrt{\varepsilon_D}} \left(\overrightarrow{\mathrm{Curl}}_{\partial D}(h_\nu E_\nu\big|_-) - \mathrm{i}\kappa \gamma_T^- H \right) \end{aligned} \tag{3.2.3}$$

and

$$\begin{aligned} \frac{1}{\sqrt{\mu_0}} \nu \times H'\big|_+ - \frac{1}{\sqrt{\mu_D}} \nu \times H'\big|_- &= \frac{1}{\sqrt{\mu_0}} \left(\overrightarrow{\mathrm{Curl}}_{\partial D}(h_\nu H_\nu|_+) + \mathrm{i}k h_\nu \gamma_T^+ E \right) \\ &\quad - \frac{1}{\sqrt{\mu_D}} \left(\overrightarrow{\mathrm{Curl}}_{\partial D}(h_\nu H_\nu|_-) + \mathrm{i}\kappa h_\nu \gamma_T^- E \right) \end{aligned} \tag{3.2.4}$$

3.3. Chiral media

In this section, we present the domain derivative for the scattering from chiral media, which is an extension of the result in [26]. Since the scattering problem is solvable for C^2 boundaries, we will always assume ∂D to be of class C^2. Let again E denote the weak solution of the scattering problem from chiral media, i.e.

$$\mathcal{C}(E, V) = \ell(V)$$

for all $V \in H(\operatorname{curl}, B_R(0))$. Let $E_h \in H(\operatorname{curl}, B_R(0))$ denote the weak solution of the scattering from chiral media with respect to the by $h \in C_0^2(B_R(0), \mathbb{R}^3)$ perturbed scatterer D_h, i.e.

$$\begin{aligned}
&\int_{B_R(0)} \Big(\frac{1}{\mu_{r,h}} - k^2 \beta_{r,h}^2 \varepsilon_{r,h}\Big) \operatorname{curl} E_h^\top \overline{\operatorname{curl} V} \,\mathrm{d}x \\
-k^2 &\int_{B_R(0)} \varepsilon_{r,h} \beta_{r,h}^2 (E_h^\top \overline{\operatorname{curl} V} + \operatorname{curl} E_h^\top \overline{V}) \,\mathrm{d}x \\
-k^2 &\int_{B_R(0)} \varepsilon_{r,h} E^\top \overline{V} \,\mathrm{d}x - \mathrm{i}k \langle \Lambda(\gamma_t E), \gamma_T V \rangle_{\partial B_R(0)} = \ell(V),
\end{aligned}$$

where $\mu_{r,h}, \varepsilon_{r,h}$ and $\beta_{r,h}$ denote the piecewise constant functions with respect to the perturbed scatterer D_h, e.g. $\beta_{r,h} = 0$ outside of D_h and $\beta_{r,h} = \beta$ inside of D_h. In contrast to the scattering from a perfect conductor, the function E_h does lie in the same function spaces as E, but the weak formulation depends implicitly on D_h, e.g. the integrals containing $\beta_{r,h}$ are effectively integrals over D_h. We again apply the transformation (3.1.2), i.e.

$$\widehat{E_h} = J_\varphi^\top \widetilde{E_h}$$

and use change of variables $x \mapsto \varphi(x) = x + h(x)$. This leads to the perturbed weak formulation

$$\mathcal{C}_h(\widehat{E_h}, V) = \ell(V) \tag{3.3.1}$$

for all $V \in H(\operatorname{curl}, B_R(0))$ with the bounded sesquilinear form

$$\mathcal{C}_h : H(\operatorname{curl}, B_R(0)) \times H(\operatorname{curl}, B_R(0)) \to \mathbb{C},$$

defined by

$$\begin{aligned}
\mathcal{C}_h(E, V) = &\int_{B_R(0)} \Big(\frac{1}{\widetilde{\mu_{r,h}}} - k^2 \widetilde{\beta_{r,h}^2} \widetilde{\varepsilon_{r,h}}\Big) \operatorname{curl} E^\top \frac{J_\varphi^\top J_\varphi}{\det(J_\varphi)} \overline{\operatorname{curl} V} \,\mathrm{d}x \\
- k^2 &\int_{B_R(0)} \widetilde{\varepsilon_{r,h}} E^\top \det(J_\varphi) J_\varphi^{-1} J_\varphi^{-\top} \overline{V} \,\mathrm{d}x \\
- k^2 &\int_{B_R(0)} \widetilde{\beta_{r,h}} \widetilde{\varepsilon_{r,h}} \big(\operatorname{curl} E^\top \overline{V} + E^\top \overline{\operatorname{curl} V}\big) \,\mathrm{d}x - \mathrm{i}k \langle \Lambda(\gamma_t E), \gamma_T V \rangle_{\partial B_R(0)}.
\end{aligned}$$

Note, that in the mixed products $\operatorname{curl} E^\top \overline{V}$ and by symmetry $E^\top \overline{\operatorname{curl} V}$, the Jacobians or its inverse of φ and the determinant $\det(\varphi)$ of the change of variables cancel due to (3.1.3). We chose the notation $\varepsilon_{r,h}, \mu_{r,h}$ and $\beta_{r,h}$, since one can extend the following results to inhomogeneous media, where these coefficients are assumed to be constant outside of D and for example differentiable and real-valued in D, see e.g. [39, Section 4.2]. Then, one can prove the following theorem in the same way, but has to consider the Taylor expansions

$$\widetilde{\beta_{r,h}}(x) = \beta_r(x) + \nabla\beta(x) \cdot h(x) + \mathcal{O}(\|h\|_{C^1}^2). \tag{3.3.2}$$

for all occurring coefficients. Since this only adds additional terms to our calculations and yields no further insight, we restrict ourselves to the case of piecewise constant coefficients μ_r, ε_r and but $\beta_r|_D \in C^1(\overline{D})$. Analogously to the perfect conductor, we can prove the following theorem.

Theorem 3.14. *Let $E \in H(\mathrm{curl}, B_R(0))$ be the solution of (2.4.12) and $\widehat{E_h} \in H(\mathrm{curl}, B_R(0))$ a solution of (3.3.1). Then we have*

$$\lim_{\|h\|_{C^1}\to 0} \|E - \widehat{E_h}\|_{H(\mathrm{curl},B_R(0)} = 0.$$

Proof. The proof is similar to the proof of Theorem 3.3. We again define bounded linear operators $C, C_h : H(\mathrm{curl}, B_R(0)) \to H(\mathrm{curl}, B_R(0))$ by the Riesz representation theorem, such that

$$\langle CE, V\rangle_{H(\mathrm{curl},B_R(0))} = \mathcal{C}(E, V), \quad \langle C_h E, V\rangle_{H(\mathrm{curl},B_R(0))} = \mathcal{C}_h(E, V)$$

for all $E, V \in H(\mathrm{curl}, B_R(0))$ and $L \in H(\mathrm{curl}, B_R(0))$ such that $\ell(V) = \langle L, V\rangle_{H(\mathrm{curl},B_R(0))}$. This leads to

$$\begin{aligned}
&\|(C_h - C)E\|_{H(\mathrm{curl},B_R(0))}^2 = \mathcal{C}_h(E, (C_h - C)E) - \mathcal{C}(E, (C_h - C)E) \\
&= \int_{B_R(0)} \mathrm{curl}\, E^\top \Big(\widetilde{\alpha_r} \frac{J_\varphi^\top J_\varphi}{\det J_\varphi} - \alpha_r I\Big) \overline{\mathrm{curl}(C_h - C)E}\, \mathrm{d}x \\
&- k^2 \int_{B_R(0)} E^\top \Big(J_\varphi^{-1} J_\varphi^{-\top} \det(J_\varphi)\widetilde{\varepsilon_{r,h}} - \varepsilon I\Big) \overline{(C_h - C)E}\, \mathrm{d}x \\
&- k^2 \int_{B_R(0)} \Big((\widetilde{\varepsilon_{r,h}}\widetilde{\beta_{r,h}} - \varepsilon_r\beta_r)\big(E^\top \overline{\mathrm{curl}(C_h - C)E} + \mathrm{curl}\, E^\top \overline{(C_h - C)E}\big)\Big)\, \mathrm{d}x
\end{aligned}$$

with $\widetilde{\alpha_r} = \frac{1}{\widetilde{\mu_{r,h}}} - k^2\widetilde{\varepsilon_{r,h}}\widetilde{\beta_{r,h}^2}$ and $\alpha_r = \frac{1}{\mu_r} - k^2\varepsilon_r\beta_{r,h}^2$. Considering the linearizations of the matrices in these integrals in the same way as in the proof of Theorem 3.3 together with the Taylor expansions of the form (3.3.2), we conclude

$$\widetilde{\varepsilon_{r,h}}\widetilde{\beta_{r,h}} - \varepsilon_r\beta_r = \varepsilon_r \nabla\beta^\top h + \mathcal{O}(\|h\|_{C^1}^2) = \mathcal{O}(\|h\|_{C^1})$$

and analogously

$$\widetilde{\alpha_r} \frac{J_\varphi^\top J_\varphi}{\det J_\varphi} - \alpha_r I = \mathcal{O}(\|h\|_{C^1(\mathbb{R}^3,\mathbb{R}^3)})$$

as well as

$$J_\varphi^{-1} J_\varphi^{-\top} \det(J_\varphi)\widetilde{\varepsilon_{r,h}} - \varepsilon_r I = \mathcal{O}(\|h\|_{C^1(\mathbb{R}^3,\mathbb{R}^3)}).$$

With the same arguments as in the proof of Theorem 3.3, we conclude

$$\|\widehat{E_h} - E\|_{H(\mathrm{curl},B_R(0))} \to 0, \quad h \to 0 \text{ in } C^1,$$

which finishes the proof. □

We continue by proving the existence of the material derivative.

Theorem 3.15. *Let ∂D be of class C^2. Let $E \in H(\mathrm{curl}, B_R(0))$ be the solution of (2.4.12) and $\widehat{E_h} \in H(\mathrm{curl}, B_R(0))$ of (3.3.1). Then there exists a function $W \in H(\mathrm{curl}, B_R(0))$, depending linearly and continuously on $h \in C^1$, such that*

$$\lim_{\|h\|_{C^1}\to 0} \frac{1}{\|h\|_{C^1}} \|\widehat{E_h} - E - W\|_{H(\mathrm{curl},B_R(0))} = 0.$$

Proof. Again, the motivation of the material derivative $W \in H(\mathrm{curl}, B_R(0))$ comes from considering the difference

$$\mathcal{C}(\widehat{E_h} - E, V) = \mathcal{C}(\widehat{E_h}, V) - \ell(V) = \mathcal{C}(\widehat{E_h}, V) - \mathcal{C}_h(\widehat{E_h}, V)$$

for any $V \in H(\mathrm{curl}, B_R(0))$. We define $W \in H(\mathrm{curl}, B_R(0))$ for a given perturbation $h \in C^1$ as the solution of

$$\begin{aligned}
\mathcal{C}(W, V) = &\int_{B_R(0)} \mathrm{curl}\, E^\top \Big(\frac{1}{\mu_r} - k^2\varepsilon_r\beta_r^2\Big)\Big(\mathrm{div}(h)I - J_h - J_h^\top\Big)\overline{\mathrm{curl}\, V}\, \mathrm{d}x \\
&+ \int_{B_R(0)} 2k^2\beta_r\varepsilon_r(\nabla\beta_r^\top h)\, \mathrm{curl}\, E^\top \overline{\mathrm{curl}\, V}\, \mathrm{d}x \\
&+ k^2 \int_{B_R(0)} \varepsilon_r E^\top \Big(\mathrm{div}(h)I - J_h - J_h^\top\Big)\overline{V}\, \mathrm{d}x \\
&+ k^2 \int_{B_R(0)} \varepsilon_r(\nabla\beta_r^\top h)(\mathrm{curl}\, E^\top \overline{V} + E^\top \overline{\mathrm{curl}\, V}\, \mathrm{d}x
\end{aligned}$$

for all $V \in H(\mathrm{curl}, B_R(0))$. Note the additional terms in comparison with the perfect conductor due to the Taylor expansion of $\widetilde{\beta_{r,h}}$ and $\widetilde{\beta_{r,h}^2}$. Similarly to Theorem 3.4, we continue by considering the difference

$$\begin{aligned}
\mathcal{C}(\widehat{E_h} - E - W, V) &= \mathcal{C}(\widehat{E_h}, V) - \ell(V) - \mathcal{C}(W, V) \\
&= \mathcal{C}(\widehat{E_h}, V) - \mathcal{C}_h(\widehat{E_h}, V) - \mathcal{C}(W, V),
\end{aligned}$$

which by adding a smart zero leads to

$$
\begin{aligned}
&\mathcal{C}(\widehat{E_h} - E - W, V) \\
&= \int_{B_R(0)} \operatorname{curl} \widehat{E_h}^\top \Big[\Big(\frac{1}{\mu_r} - k^2\beta_r^2\varepsilon_r\Big)\big(I - \operatorname{div}(h)I + J_h + J_h^\top\big) \\
&\qquad - 2k^2\varepsilon_r\beta_r(\nabla\beta^\top h)I - \Big(\frac{1}{\widetilde{\mu_{r,h}}} - k^2\widetilde{\varepsilon_{r,h}}\widetilde{\beta_{r,h}^2}\Big)\frac{J_\varphi^\top J_\varphi}{\det J_\varphi}\Big]\overline{\operatorname{curl} V}\,\mathrm{d}x \\
&- k^2\int_{B_R(0)} \widehat{E_h}\big(\varepsilon_r(I + \operatorname{div}(h)I - J_h - J_h^\top) - \widetilde{\varepsilon_{r,h}}J_\varphi^{-1}J_\varphi^{-\top}\det J_\varphi\big)\overline{V}\,\mathrm{d}x \\
&- k^2\int_{B_R(0)} \big(\beta_r\varepsilon_r + \varepsilon_r(\nabla\beta^\top h) - \widetilde{\varepsilon_{r,h}}\widetilde{\beta_{r,h}}\big)\big(\operatorname{curl}\widehat{E_h}^\top\overline{V} + \widehat{E_h}^\top\overline{\operatorname{curl} V}\big)\,\mathrm{d}x \\
&+ \int_{B_R(0)} \operatorname{curl}(\widehat{E_h} - E)^\top\Big[\Big(\frac{1}{\mu_r} - k^2\varepsilon_r\beta_r^2\Big)\big(\operatorname{div}(h)I - J_h - J_h^\top\big) \\
&\qquad + 2k^2\varepsilon_r\beta_r(\nabla\beta^\top h)\Big)\Big]\overline{\operatorname{curl} V}\,\mathrm{d}x \\
&+ k^2\int_{B_R(0)} (\widehat{E_h} - E)^\top\big(\varepsilon_r(\operatorname{div}(h)I - J_h - J_h^\top)\big)\overline{V}\,\mathrm{d}x \\
&+ k^2\int_{B_R(0)} (\varepsilon_r\nabla\beta^\top h)\big((\widehat{E_h} - E)^\top\overline{\operatorname{curl} V} + \operatorname{curl}(\widehat{E_h} - E)^\top\overline{V}\big)\,\mathrm{d}x.
\end{aligned}
$$

Using the linearizations from Lemma 3.2 and the Taylor expansion of $\widetilde{\beta_r}$ together with Cauchy-Schwarz leads to

$$
\begin{aligned}
\mathcal{C}(\widehat{E_h} - E - W, V) \leqslant C\big[&\|\widehat{E_h}\|_{H(\operatorname{curl},B_R(0))}\mathcal{O}(\|h\|_{C^1}^2) \\
&+ \|\widehat{E_h} - E\|_{H(\operatorname{curl},B_R(0))}\mathcal{O}(\|h\|_{C^1})\big]\|V\|_{H(\operatorname{curl},B_R(0))}
\end{aligned}
$$

for some constant $C > 0$. With the previous theorem, we conclude

$$
\frac{1}{\|h\|_{C^1}}\|\widehat{E_h} - E - W\|_{H(\operatorname{curl},B_R(0))} \to 0
$$

for $h \to 0$ in C^1, which finishes the proof. $\square$

The function $W \in H(\operatorname{curl}, B_R(0))$ is again called *material derivative* of E with respect to the perturbation h. We can again extract the *domain derivative* E', as the following theorem shows.

Theorem 3.16. *Let ∂D be of class C^2. In the setting of Theorem 3.15, we define $E' = W - J_h^\top E - J_E h$. Then $E'|_D \in H(\operatorname{curl}, D)$ and $E'|_{B_R(0)\setminus\overline{D}} \in$*

$H(\operatorname{curl}, B_R(0) \setminus \overline{D}$ can be uniquely extended to the radiating weak solution of the scattering problem from chiral media, i.e.

$$\operatorname{curl} E' = \mathrm{i}k\mu_r(H' + \beta_r \operatorname{curl} H'), \quad \operatorname{curl} H' = -\mathrm{i}k\varepsilon_r(E' + \beta_r \operatorname{curl} E') \quad \text{in } \mathbb{R}^3 \setminus \overline{\partial D}$$

where H' is defined by a combination of these equations. E' and H' satisfy the transmission boundary conditions

$$[\nu \times E']_\pm = \left[\overrightarrow{\operatorname{Curl}}_{\partial D}(h_\nu E_\nu) - h_\nu(\nu \times (\operatorname{curl} E \times \nu))\right]_\pm$$
$$[\nu \times H']_\pm = \left[\overrightarrow{\operatorname{Curl}}_{\partial D}(h_\nu H_\nu) + h_\nu(\nu \times (\operatorname{curl} H \times \nu))\right]_\pm .$$

Proof. The proof is similar to the proof of Theorem 3.6 and an extension of [26, Theorem 4.1]. First, the regularity of ∂D yields classic smooth solutions $E|_D, H|_D \in C^1(D, \mathbb{C}^3) \cap C(\overline{D}, \mathbb{C}^3)$ and $E|_{B_R(0)\setminus\overline{D}}, H|_{B_R(0)\setminus\overline{D}} \in C^1(B_R(0) \setminus \overline{D}, \mathbb{C}^3) \cap C(B_R(0) \setminus D)$, see [5, Theorem 3]. Therefore $E' = W - J_h^\top E - J_E h \in L^2(B_R(0))$ is well defined. By considering again

$$\operatorname{curl}\left(J_h^\top E + J_E h\right) = \operatorname{div}(h) \operatorname{curl} E + J_{\operatorname{curl} E} - J_h \operatorname{curl} E$$

we conclude $E'|_D \in H(\operatorname{curl}, D)$ and $E'|_{B_R(0)\setminus\overline{D}} \in H(\operatorname{curl}, B_R(0) \setminus \overline{D})$, since by combining the Maxwell system in chiral media (2.4.9a), we have

$$(1 - k^2\mu_r\varepsilon_r\beta_r^2) \operatorname{curl} E = \mathrm{i}k\mu_r H + k^2\mu_r\varepsilon_r\beta_r E$$

and therefore differentiability of $\operatorname{curl} E$ inside of D and in $B_R(0)\setminus\overline{D}$. Similarly to the characterization of the domain derivative for the scattering from a perfect conductor, we consider the difference

$$\begin{aligned}
&\mathcal{C}(E', V) = \mathcal{C}(W, V) - \mathcal{C}(J_h^\top E + J_E h, V) \\
&= \int_{B_R(0)} \operatorname{curl} E^\top \Big(\alpha_r(\operatorname{div}(h) I - J_h - J_h^\top) + 2k^2\varepsilon_r\beta_r(\nabla\beta_r^\top h) I\Big) \overline{\operatorname{curl} V} \,\mathrm{d}x \\
&\quad + k^2 \int_{B_R(0)} \varepsilon_r E^\top(\operatorname{div}(h) I - J_h - J_h^\top)\overline{V} \,\mathrm{d}x \\
&\quad + k^2 \int_{B_R(0)} \varepsilon_r(\nabla\beta_r^\top h)(\operatorname{curl} E^\top \overline{V} + E^\top \overline{\operatorname{curl} V} \,\mathrm{d}x \\
&\quad - \int_{B_R(0)} \alpha_r \operatorname{curl}(J_h^\top E + J_E h)^\top \overline{\operatorname{curl} V} + k^2 \int_{B_R(0)} \varepsilon_r (J_h^\top E + J_E h)^\top \overline{V} \,\mathrm{d}x \\
&\quad + k^2 \int_{B_R(0)} \varepsilon_r\beta_r\big(\operatorname{curl}(J_h^\top E + J_E h)^\top \overline{V} + (J_h^\top E + J_E h)^\top \overline{\operatorname{curl} V} \,\mathrm{d}x,
\end{aligned} \tag{3.3.3}$$

where again $\alpha_r = \frac{1}{\mu_r} - k^2\beta_r^2\varepsilon_r$. Note the vanishing boundary integrals on $\partial B_R(0)$ of the second term, due to the compact support of h in $B_R(0)$. We are going to summarize these terms. In order to keep track of all terms, we introduce the notation

$$\mathcal{C}(E', V) =: \int_{B_R(0)} \left(T_1^\top \overline{\operatorname{curl} V} + T_2^\top \overline{V} \right) \mathrm{d}x, \tag{3.3.4}$$

where the terms T_1 and T_2 are implicitly defined such that equations (3.3.3) and (3.3.4) are the same. We start by simplifying the integrals containing T_2. We are using

$$\operatorname{curl}(J_h^\top E + J_E h) = \operatorname{curl}(\operatorname{curl} E \times h) \quad \text{and} \quad \nabla(h^\top E) = J_h^\top E + J_E^\top h, \tag{3.3.5}$$

which yields

$$\begin{aligned}\int_{B_R(0)} \overline{V}^\top T_2 \,\mathrm{d}x = k^2 \int_{B_R(0)} \varepsilon_r \overline{V}^\top \Big[&(\operatorname{div}(h) I - J_h - J_h^\top) E \\ &+ (\nabla\beta_r^\top h) \operatorname{curl} E + \nabla(h^\top E) + (J_E - J_E^\top) h + \beta_r \operatorname{curl}(\operatorname{curl} E \times h) \Big] \,\mathrm{d}x.\end{aligned}$$

We further use

$$(J_E - J_E^\top) h = \operatorname{curl} E \times h$$

and

$$\operatorname{curl}(E \times h) = \operatorname{div}(h) E - \operatorname{div}(E) h + J_E h - J_h E$$

to get

$$\begin{aligned}\int_{B_R(0)} \overline{V}^\top T_2 \,\mathrm{d}x = k^2 \int_{B_R(0)} \varepsilon_r \overline{V}^\top \Big[&\operatorname{curl}(E \times h) + \operatorname{div}(E) h - J_E h - J_h^\top E \\ &+ (\nabla\beta_r^\top h) \operatorname{curl} E + \nabla(h^\top E) + \operatorname{curl} E \times h + \beta_r \operatorname{curl}(\operatorname{curl} E \times h) \Big] \,\mathrm{d}x.\end{aligned}$$

Using again

$$-J_E h - J_h^\top E = -\nabla(h^\top E) - \operatorname{curl} E \times h$$

we arrive at

$$\begin{aligned}\int_{B_R(0)} \overline{V}^\top T_2 \,\mathrm{d}x = k^2 \int_{B_R(0)} \varepsilon_r \overline{V}^\top \Big(&\operatorname{curl}(E \times h) + \operatorname{div}(E) h \\ &+ (\nabla\beta_r^\top h) \operatorname{curl} E + \beta_r \operatorname{curl}(\operatorname{curl} E \times h) \Big) \,\mathrm{d}x.\end{aligned}$$

Considering the formula

$$\operatorname{curl}(A \times B) = A \operatorname{div}(B) - \operatorname{div}(A)B + J_A B - J_B A \tag{3.3.6}$$

for vector fields A and B together with the product rule for the Jacobian of the product of some scalar function α_r and a vector field B

$$J_{\alpha_r A} = \alpha_r J_A + A J_{\alpha_r} = \alpha_r J_A + A \nabla\alpha_r^\top,$$

we find

$$\operatorname{curl}(\beta \operatorname{curl} E \times h) = \beta \operatorname{curl}(\operatorname{curl} E \times h) - (\operatorname{curl} E^\top \nabla\beta_r)h + (\operatorname{curl} E \nabla\beta_r^\top)h.$$

Note $(\nabla\beta_r^\top h) \operatorname{curl} E = (\operatorname{curl} E \nabla\beta_r^\top)h$. From Maxwell's equations in chiral media, we see

$$\operatorname{div}(E) = -\nabla\beta_r^\top \operatorname{curl} E.$$

This leads finally to

$$\int_{B_R(0)} \overline{V}^\top T_2 \, \mathrm{d}x = k^2 \int_{B_R(0)} \varepsilon_r \operatorname{curl}\big((E + \beta \operatorname{curl} E) \times h\big)^\top \overline{V} \, \mathrm{d}x.$$

Now, we consider the integral

$$\begin{aligned}
&\int_{B_R(0)} \overline{\operatorname{curl} V}^\top T_1 \, \mathrm{d}x \\
&= \int_{B_R(0)} \overline{\operatorname{curl} V}^\top \Big[\alpha_r\big(\operatorname{div}(h)I - J_h - J_h^\top\big) \operatorname{curl} E \\
&\qquad + 2k^2 \varepsilon_r \beta_r (\nabla\beta_r^\top h) \operatorname{curl} E + k^2 \varepsilon_r (\nabla\beta_r^\top h) E \\
&\qquad - \alpha_r \operatorname{curl}(J_h^\top E + J_E h) + k^2 \varepsilon_r \beta_r (J_h^\top E + J_E h)\Big] \, \mathrm{d}x.
\end{aligned}$$

First, we use again (3.3.5), which yields

$$\begin{aligned}
&\int_{B_R(0)} \overline{\operatorname{curl} V}^\top T_1 \, \mathrm{d}x \\
&= \int_{B_R(0)} \Big[\alpha_r\big(\operatorname{div}(h)I - J_h - J_h^\top\big) \operatorname{curl} E \\
&\quad + k^2 \varepsilon_r \beta_r (\nabla\beta_r^\top h) \operatorname{curl} E + k^2 \varepsilon_r (\nabla\beta_r^\top h) E \\
&\quad - \alpha_r \operatorname{curl}(\operatorname{curl} E \times h) + \varepsilon_r \beta_r k^2 \nabla(h^\top E) + k^2 \varepsilon_r \beta_r \operatorname{curl} E \times h\Big] \, \mathrm{d}x
\end{aligned}$$

With (3.3.6) we find

$$\operatorname{div}(h)\operatorname{curl}E - J_h^\top \operatorname{curl}E + J_{\operatorname{curl}E}h = \operatorname{curl}(\operatorname{curl}E \times h)$$

and therefore

$$\begin{aligned}
&\int_{B_R(0)} \overline{\operatorname{curl}V}^\top T_1 \,\mathrm{d}x \\
&= \int_{B_R(0)} \overline{\operatorname{curl}V}^\top \Big[\alpha_r\big(- J_h^\top \operatorname{curl}E - J_{\operatorname{curl}E}h\big) + 2k^2\varepsilon_r\beta_r(\nabla\beta_r^\top h)\operatorname{curl}E \\
&\quad + k^2\varepsilon_r(\nabla\beta_r^\top h)E + k^2\beta_r\varepsilon_r\nabla(h^\top E) + k^2\varepsilon_r\beta_r\operatorname{curl}E\times h\Big]\,\mathrm{d}x.
\end{aligned}$$

We continue by considering

$$\begin{aligned}
&\alpha_r(-J_h^\top \operatorname{curl}E - J_{\operatorname{curl}E}h) = -\alpha_r\nabla(h^\top\operatorname{curl}E) - \alpha_r\operatorname{curl}\operatorname{curl}E\times h \\
&= - \nabla\big(\alpha_r(h^\top\operatorname{curl}E)\big) + (h^\top\operatorname{curl}E)\nabla\alpha_r \\
&\quad - \operatorname{curl}(\alpha_r\operatorname{curl}E)\times h + (\nabla\alpha_r\times\operatorname{curl}E)\times h \\
&= - \nabla\big(\alpha_r(h^\top\operatorname{curl}E)\big) - \operatorname{curl}(\alpha_r\operatorname{curl}E)\times h + (\nabla\alpha_r^\top h)\operatorname{curl}E.
\end{aligned}$$

Recall $\alpha_r = \frac{1}{\mu_r} - k^2\varepsilon_r\beta_r^2$ and therefore $\nabla\alpha_r = -2k^2\varepsilon_r\beta_r\nabla\beta_r$. Instead of considering the first order system (2.4.9a) for the two unknown solutions E and H, one can consider the following second order partial differential equation, where only the electric field appears:

$$\operatorname{curl}\big(\alpha_r\operatorname{curl}E\big) - k^2\varepsilon_r E - k^2\varepsilon_r\beta_r\operatorname{curl}E - k^2\varepsilon_r\operatorname{curl}(\beta_r E) = 0. \tag{3.3.7}$$

This can be achieved by plugging the second equation from (2.4.9a) into the first, then applying the curl operator and again using the second equation from (2.4.9a). One can easily see, that the weak formulation of this second order partial differential equation is again given by the bounded sesquilinear form $\mathcal{C}$. We need this strong formulation to continue our calculations. Using (3.3.7), we find

$$\begin{aligned}
&\alpha_r(-J_h^\top\operatorname{curl}E - J_{\operatorname{curl}E}h) \\
&= - \nabla\big(\alpha_r(h^\top\operatorname{curl}E)\big) + (\nabla\alpha_r^\top h)\operatorname{curl}E - k^2\varepsilon_r E\times h \\
&\quad - k^2\varepsilon_r\beta_r\operatorname{curl}E\times h - k^2\varepsilon_r\operatorname{curl}(\beta_r E)\times h
\end{aligned}$$

Together with

$$\operatorname{curl}(\beta_r E)\times h = \beta_r\operatorname{curl}E\times h + \big(\nabla\beta_r\times E\big)\times h$$

$$=\beta_r \operatorname{curl} E \times h - (h^\top E)\nabla\beta_r + \big(\nabla\beta_r^\top h\big)E$$

we arrive at

$$\begin{aligned}
&\int_{B_R(0)} \overline{\operatorname{curl} V}^\top T_1 \,\mathrm{d}x \\
&= \int_{B_R(0)} \overline{\operatorname{curl} V}^\top \Big[-\nabla(\alpha_r(h^\top \operatorname{curl} E)) + k^2\beta_r\varepsilon_r\nabla(h^\top E) + k^2\varepsilon_r\beta_r \operatorname{curl} E \times h \\
&\qquad - k^2\varepsilon_r(E\times h) - 2k^2\varepsilon_r\beta_r \operatorname{curl} E \times h + k^2\varepsilon_r(h^\top E)\nabla\beta_r\Big] \,\mathrm{d}x \\
&= \int_{B_R(0)} \overline{\operatorname{curl} V}^\top \Big[\nabla(h^\top(k^2\varepsilon_r\beta_r E - \alpha_r \operatorname{curl} E)) \\
&\qquad - k^2\varepsilon_r(E+\beta_r \operatorname{curl} E)\times h\Big] \,\mathrm{d}x.
\end{aligned}$$

Recalling (3.3.4), we finally have

$$\begin{aligned}
\mathcal{C}(E', V) = &\int_{B_R(0)} \overline{V}^\top \Big(k^2\varepsilon_r \operatorname{curl}\big((E+\beta_r \operatorname{curl} E)\times h\big)\Big) \,\mathrm{d}x \\
&+ \int_{B_R(0)} \overline{\operatorname{curl} V}^\top \Big(\nabla\big(h^\top(k^2\varepsilon_r\beta_r E - \alpha_r \operatorname{curl} E)\big) \\
&\qquad - k^2\varepsilon_r(E+\beta_r \operatorname{curl} E)\times h\Big) \,\mathrm{d}x.
\end{aligned}$$

Using the identities

$$\nabla f^\top \operatorname{curl} G = \operatorname{div}(f \operatorname{curl} G) \quad \text{and} \quad \operatorname{div}(F\times G) = \operatorname{curl} F^\top G - F^\top \operatorname{curl} G$$

for some scalar function f and vector fields F and G, we get

$$\begin{aligned}
\mathcal{C}(E', V) = \int_{B_R(0)} &\Big(\operatorname{div}\big[\big(h^\top(k^2\varepsilon_r\beta_r E - \alpha_r \operatorname{curl} E)\big)\overline{\operatorname{curl} V}\big] \\
&\qquad + \operatorname{div}\big[k^2\varepsilon_r\big((E+\beta_r \operatorname{curl} E)\times h\big)\times \overline{V}\big]\Big) \,\mathrm{d}x.
\end{aligned}$$

Now, we can apply the Theorem of Gauß. Note, that due to the discontinuities of α_r, ε_r and β_r, we have to apply the theorem in D and in $B_R(0)$. Since h is compactly supported in $B_R(0)$, no boundary integrals on $\partial B_R(0)$ occur. This leads to

$$\mathcal{C}(E', V) = \int_{\partial D} \Big[\big(h^\top(k^2\varepsilon_r\beta_r E - \alpha_r \operatorname{curl} E)\big)\nu^\top \overline{\operatorname{curl} V}$$

$$- k^2\varepsilon_r\nu^\top\Big(\big((E+\beta_r\operatorname{curl}E)\times h\big)\times\overline{V}\Big)\Big]_\pm\,\mathrm{d}s. \quad (3.3.8)$$

From the definition of the weak formulation (2.4.10) and (2.4.11), we see that E' is a solution of the scattering problem from chiral media that satisfies the radiation condition. Comparing (2.4.10) to (3.3.8), we see

$$\mathcal{C}(E',V) = -\mathrm{i}k\int_{\partial D}[\nu\times H']_\pm^\top\big(\nu\times(\overline{V}\times\nu)\big)\,\mathrm{d}s.$$

Combining equations (2.2.5) and (2.2.6), we have

$$\int_{\partial D} u\nu^\top\operatorname{curl}F\,\mathrm{d}s = \int_{\partial D}\operatorname{Grad}_{\partial D}u^\top(\nu\times F)\,\mathrm{d}s$$

and therefore with $(a\times b)^\top c = -(c\times b)^\top a$ we find

$$\mathcal{C}(E',V) = \int_{\partial D}\big[\operatorname{Grad}_{\partial D}\big(h^\top(k^2\varepsilon_r\beta_r E-\alpha_r\operatorname{curl}E)\big) \\ + k^2\varepsilon_r(E+\beta_r\operatorname{curl}E)\times h\big]_\pm^\top(\nu\times\overline{V})\,\mathrm{d}s.$$

From Maxwell's equations in chiral material, we have

$$\mathrm{i}kH = \alpha_r\operatorname{curl}E - k^2\varepsilon_r\beta_r E \quad\text{and}\quad \operatorname{curl}H = -\mathrm{i}k\varepsilon_r(E+\beta_r\operatorname{curl}E),$$

which leads to

$$\mathcal{C}(E',V) = -\mathrm{i}k\int_{\partial D}\big[\operatorname{Grad}_{\partial D}(h^\top H) - \operatorname{curl}H\times h\big]_\pm^\top(\nu\times\overline{V})\,\mathrm{d}s.$$

Considering the expansion

$$H = H_\tau + H_\nu\nu = (\nu\times(H\times\nu)) + (H\cdot\nu)\nu$$

and since $[\nu\times H]_\pm = 0$, we have $\operatorname{Grad}_{\partial D}(h^\top H) = \operatorname{Grad}_{\partial D}(h_\nu H_\nu)$. This leads to

$$\mathcal{C}(E',V) = -\mathrm{i}k\int_{\partial D}\big[-\nu\times\operatorname{Grad}(h_\nu H_\nu) + \nu\times(\operatorname{curl}H\times h)\big]_\pm^\top(\nu\times(\overline{V}\times\nu))\,\mathrm{d}s.$$

Recall $\overrightarrow{\operatorname{Curl}}_{\partial D}\cdot = \operatorname{Grad}_{\partial D}\cdot\times\nu$. Finally, we compute

$$\begin{aligned}[\nu\times(\operatorname{curl}H\times h)]_\pm &= [h_\nu\operatorname{curl}H]_\pm - [h(\operatorname{curl}H)_\nu]_\pm \\ &= h_\nu[\operatorname{curl}H)]_\pm + h_\tau[\operatorname{Div}_{\partial D}\nu\times H]_\pm = h_\nu[\operatorname{curl}H)]_\pm.\end{aligned}$$

With this, we conclude

$$[\nu \times H']_\pm = \left[\overrightarrow{\operatorname{Curl}}_{\partial D}(h_\nu H_\nu) + h_\nu(\nu \times (\operatorname{curl} H \times \nu))\right]_\pm.$$

Since $[\nu \times W]_\pm = 0$ on ∂D, we have

$$[\nu \times E']_\pm = -\left[\nu \times (J_E h + J_h^\top E)\right]_\pm.$$

Using $J_E h + J_h^\top E = \operatorname{curl} E \times h + \nabla(h^\top E)$ together with $[\nu \times E]_\pm = 0$ we conclude

$$[\nu \times E']_\pm = \left[\overrightarrow{\operatorname{Curl}}_{\partial D}(h_\nu E_\nu) - h_\nu(\nu \times (\operatorname{curl} E \times \nu))\right]_\pm.$$

□

This result is in line with Theorem 3.13 from Section 3.2, the domain derivative for penetrable obstacle, since we have $\operatorname{curl} E = -\mathrm{i}\kappa H$ and $\operatorname{curl} H = \mathrm{i}\kappa E$ and $\operatorname{curl} E = -\mathrm{i}kH$ in D and $\operatorname{curl} H = \mathrm{i}kE$ in $\mathbb{R}^3 \setminus \overline{D}$ if $\beta_r \equiv 0$. The remaining difference is due to the different scaling of the solutions.

3.4. Obstacles with impedance boundary condition

In this section, we present the domain derivative for the scattering from an bounded obstacle with impedance boundary condition. We extend the techniques used in [26] and in [25], for which boundaries of class C^2 are needed. The higher regularity is needed for two reasons. First, the weak formulation involves boundary integrals on ∂D. In order to linearize the deformation of such integrals and, the boundary has to be at least of class C^2. In order to characterize the domain derivative, we need again the solution to be in H^1 and therefore the boundary to at least of class C^1. Our actual calculations rely heavily on equations formulated in [40], where regular boundaries are assumed. Here, lower regularity assumptions might be possible. Let again $E \in H_{\text{imp}}(\Omega)$ denote the weak solution of the scattering problem, i.e.

$$\mathcal{B}(E, V) = \ell(V)$$

for all $V \in H_{\text{imp}}(\Omega)$, see (2.4.8) in Section 2.4.2. Let $E_h \in H_{\text{imp}}(\Omega_h)$ denote the weak solution of the scattering problem with respect to the perturbed scatterer D_h, i.e.

$$\int_{\Omega_h} \left(\operatorname{curl} E_h^\top \overline{\operatorname{curl} V} - k^2 E_h^\top \overline{V}\right) \mathrm{d}x - \mathrm{i}k\langle \Lambda \gamma_t E_h, \gamma_T V\rangle_{\partial B_R(0)}$$

$$- \mathrm{i}k \int_{\partial D_h} \lambda (\nu_h \times E_h)^\top (\nu_h \times \overline{V}) \, \mathrm{d}s = \ell(V). \quad (3.4.1)$$

We have to comment on the regularity of the impedance $\lambda : \partial D \to \mathbb{R}$. By perturbing the boundary ∂D, we have to define $\lambda : \partial D_h \to \mathbb{R}$. Since any $y \in \partial D_h$ is given by $y = x + h(x)$ for exactly one $x \in \partial D$, one could define $\lambda(y = x + h(x)) = \lambda(x)$. This case has been considered in [10]. We want to consider the more general setting, where we also allow λ to change. Therefore we will assume from now on $\lambda \in C^1(\mathbb{R}^3)$.

Note, that in contrast to the scattering from a perfect conducting or penetrable obstacle, we have to consider the additional integral over the surface ∂D_h. With $\nu_h : \partial D_h \to \mathbb{S}^2$, we denote the outwards drawn normal vector field with respect to ∂D_h. The normal vectors of ∂D and ∂D_h are related. This is illustrated by the following lemma.

Lemma 3.17. *Let ∂D be of class C^1. Let $x \in \partial D$ and $\nu(x)$ the normal vector of ∂D at x. Let further $\nu_h(\varphi(x))$ be the normal vector of ∂D_h at $\varphi(x) = x + h(x)$. Then*

$$\nu_h(x + h(x)) = \nu_h(\varphi(x)) = \frac{J_\varphi^{-\top} \nu(x)}{|J_\varphi^{-\top} \nu(x)|}.$$

Proof. Let $\Phi : S \subset \mathbb{R}^2 \to \partial D$ be a local parametrization of ∂D with $\Phi(0) = x$. We can define by

$$\widehat{\Phi} : S \to \mathbb{R}^3, \quad \widehat{\Phi}(\hat{x}) = \Phi(\hat{x}) + h(\Phi(\hat{x}))$$

a local parametrization of ∂D_h with $\widehat{\Phi}(0) = x + h(x)$. We define

$$\hat{\nu} := J_\varphi^{-\top} \nu(x)$$

and claim $\hat{\nu}$ to be orthogonal to ∂D_h at $x + h(x)$. By the chain rule, we compute for $i \in \{1, 2\}$

$$\frac{\partial \widehat{\Phi}}{\partial x_i}(0) = \frac{\partial \Phi}{\partial x_i}(0) + J_h(\Phi(\hat{x}))\frac{\partial \Phi}{\partial x_i}(0) = (I + J_h(x))\frac{\partial \Phi}{\partial x_i}(0) = J_\varphi(x)\frac{\partial \Phi}{\partial x_i}(0).$$

Therefore, we have

$$\hat{\nu} \cdot \frac{\partial \widehat{\Phi}}{\partial x_i}(0) = \nu(x)^\top J_\varphi^{-1}(x) J_\varphi(x) \frac{\partial \Phi}{\partial x_i}(0) = \nu(x) \cdot \frac{\partial \Phi}{\partial x_i}(0) = 0,$$

for $i = 1, 2$, since $\frac{\partial \Phi}{\partial x_i}(0)$ is a tangential vector at $x = \Phi(0)$. Additionally, $\hat{\nu}$ is outwards directed, since $\hat{\nu} \to \nu$ for $h \to 0$ and $\hat{\nu}$ depends continuously on h. Therefore, $\hat{\nu}$ is up to normalization the claimed normal vector. $\square$

We employ again the change of variables $x \mapsto \varphi(x)$ to transform the integrals over Ω_h in (3.4.1) to integrals over Ω. For the surface integral on ∂D_h, we define the *surface functional determinant* $\operatorname{Det}\varphi$ implicitly by

$$\int_{\partial D_h} \mathrm{d}s = \int_{\partial D} \operatorname{Det}\varphi \,\mathrm{d}s,$$

see [25, Section 2.3]. If $\Phi : S \subset \mathbb{R}^3$ is a global parametrization of ∂D, i.e. $\Phi(S) = \partial D$ and $\widehat{\Phi} : S \subset \mathbb{R}^3$ of ∂D_h, i.e. $\widehat{\Phi} = \Phi + h \circ \Phi$, then one finds the explicit representation of $\operatorname{Det}\varphi$ in local coordinates by considering

$$\begin{aligned}\int_{\partial D_h} \mathrm{d}s &= \int_S \Big| \frac{\partial \widehat{\Phi}}{\partial x_1}(x) \times \frac{\partial \widehat{\Phi}}{\partial x_2}(x) \Big| \,\mathrm{d}x \\ &= \int_S \underbrace{\frac{\Big|\frac{\partial \widehat{\Phi}}{\partial x_1}(x) \times \frac{\partial \widehat{\Phi}}{\partial x_2}(x)\Big|}{\Big|\frac{\partial \Phi}{\partial x_1}(x) \times \frac{\partial \Phi}{\partial x_2}(x)\Big|}}_{=:\operatorname{Det}\varphi} \Big| \frac{\partial \Phi}{\partial x_1}(x) \times \frac{\partial \Phi}{\partial x_2}(x) \Big| \,\mathrm{d}x = \int_{\partial D} \operatorname{Det}\varphi \,\mathrm{d}s.\end{aligned}$$

For non global parametrizations, one defines $\operatorname{Det}\varphi$ using a partition of unity in a point $x \in \partial D$ by the above fraction for any parametrization which maps to x. We will see, that this definition does not depend on the choice of the parametrization.

We use again the transformation (3.1.3)

$$\widehat{E_h} = J_\varphi^\top \widetilde{E_h}.$$

Note that the proof of Lemma 3.1 yields $\widehat{E_h} \in H_{\mathrm{imp}}(\Omega)$. The boundary integral in (3.4.1) transforms then with Lemma 3.17 as follows

$$\begin{aligned}\int_{\partial D_h} \lambda(\nu_h \times E_h)^\top (\nu_h \times V_h) \,\mathrm{d}s &= \int_{\partial D} \widetilde{\lambda}(\widetilde{\nu_h} \times \widetilde{E_h})^\top (\widetilde{\nu_h} \times \widetilde{V_h}) \operatorname{Det}\varphi \,\mathrm{d}s \\ &= \int_{\partial D} \widetilde{\lambda}(J_\varphi^{-\top}\nu \times J_\varphi^{-\top}\widehat{E_h})^\top (J_\varphi^{-\top}\nu \times J_\varphi^{-\top}\widehat{V_h}) \frac{\operatorname{Det}\varphi}{|J_\varphi^{-\top}\nu|^2} \,\mathrm{d}s.\end{aligned}$$

We use the identity

$$(Au) \times (Av) = \det(A) A^{-\top}(u \times v)$$

for an invertible matrix $A \in \mathbb{R}^{3\times 3}$ and $u, v \in \mathbb{R}^3$, which can be seen from

$$\big((Au) \times (Av)\big) \cdot w = \det(Au|Av|w) = \det(A)\det(u|v|A^{-1}w)$$

$$= \det(A)(u \times v) \cdot (A^{-1}w) = \det(A)\big(A^{-\top}(u \times v)\big) \cdot w,$$

to get

$$\int_{\partial D_h} \lambda(\nu_h \times E_h)^\top(\nu_h \times V_h)\,\mathrm{d}s$$
$$= \int_{\partial D} \widetilde{\lambda}(\nu \times \widehat{E_h})^\top J_\varphi^\top J_\varphi(\nu \times \widehat{V_h})\frac{\operatorname{Det}\varphi}{\det(J_\varphi)^2|J_\varphi^{-\top}\nu|^2}\,\mathrm{d}s.$$

The following lemma helps us to simplify the last term and shows, that the Definition of the surface functional determinant $\operatorname{Det}(\varphi)$ does not depend on the chosen parametrization.

Lemma 3.18. *Let ∂D be of class C^1. Then we have*

$$\frac{\operatorname{Det}\varphi}{\det J_\varphi |J_\varphi^{-\top}\nu|} \equiv 1 \quad \text{on } \partial D.$$

Proof. Recall the proof of Lemma 3.1. There we have shown, that the following holds:

$$\int_{\partial D_h} \gamma_t E_h^\top \gamma_T V_h\,\mathrm{d}s = \int_{\partial D} \gamma_t \widehat{E_h}^\top \gamma_T \widehat{V_h}\,\mathrm{d}s.$$

On the other hand, we have

$$\int_{\partial D_h} \gamma_t E_h^\top \gamma_T V_h\,\mathrm{d}s = \int_{\partial D_h} (\nu_h \times E_h)^\top V_h\,\mathrm{d}s = \int_{\partial D} (\widetilde{\nu_h} \times \widetilde{E_h})^\top \widetilde{V_h} \operatorname{Det}\varphi\,\mathrm{d}s$$
$$= \int_{\partial D} (J_\varphi^{-\top}\nu \times J_\varphi^{-\top}\widehat{E_h})^\top (J_\varphi^{-\top}\widehat{V_h})\frac{\operatorname{Det}\varphi}{|J_\varphi^{-\top}\nu|}\,\mathrm{d}s$$
$$= \int_{\partial D} (\nu \times \widehat{E_h})^\top \widehat{V_h}\frac{\operatorname{Det}\varphi}{\det J_\varphi |J_\varphi^{-\top}\nu|}\,\mathrm{d}s.$$

So we conclude

$$\frac{\operatorname{Det}\varphi}{\det J_\varphi |J_\varphi^{-\top}\nu|} \equiv 1.$$

□

Note, that we have shown

$$\operatorname{Det}(\varphi) = \det(J_\varphi)|J_\varphi^{-\top}\nu|,$$

an explicit representation of the surface functional determinant.

In conclusion, we have shown that $E_h \in H_{\mathrm{imp}}(\Omega_h)$ is a weak solution of the scattering from the perturbed scatterer D_h if and only if $\widehat{E_h} \in H_{\mathrm{imp}}(\Omega)$ is a solution of

$$\int_\Omega \left(\operatorname{curl} \widehat{E_h}^\top \frac{J_\varphi^\top J_\varphi}{\det J_\varphi} \overline{\operatorname{curl} V} - k^2 \widehat{E_h}^\top \det J_\varphi J_\varphi^{-1} J_\varphi^{-\top} \overline{V} \right) \mathrm{d}x$$
$$- \mathrm{i}k \int_{\partial D} \widetilde{\lambda} \gamma_t \widehat{E_h}^\top \frac{J_\varphi^\top J_\varphi}{\operatorname{Det} \varphi} \overline{\gamma_t V} \,\mathrm{d}s + \mathrm{i}k \langle \Lambda(\gamma_t \widehat{E_h}), \gamma_T V \rangle_{\partial B_R(0)} = \ell(V) \quad (3.4.2)$$

for all $V \in H_{\mathrm{imp}}(\Omega)$. We define the bounded sesquilinear form

$$\mathcal{B}_h : H_{\mathrm{imp}}(\Omega) \times H_{\mathrm{imp}}(\Omega) \to \mathbb{C}$$

such that (3.4.2) reads as

$$\mathcal{B}_h(\widehat{E_h}, V) = \ell(V) \quad \text{for all } V \in H_{\mathrm{imp}}(\Omega). \quad (3.4.3)$$

To investigate the behaviour of $\widehat{E_h}$ as $h \to 0$ in C^1, we need the following additional linearization.

Lemma 3.19. *Let ∂D be of class C^2 and let $\lambda \in C^1(\mathbb{R}^3)$. Then*

$$\frac{\widetilde{\lambda}}{\operatorname{Det} \varphi} = \lambda(1 - \operatorname{Div}_{\partial D}(h_\tau) - 2\kappa h_\nu) + \nabla \lambda^\top h + \mathcal{O}(\|h\|^2_{C^1(\mathbb{R}^3,\mathbb{R}^3)})$$

for $h \to 0$ in C^1.

Proof. By Lemma 3.18, we have

$$\operatorname{Det}(\varphi) = \det J_\varphi |J_\varphi^{-\top} \nu|.$$

From the proof of Lemma 3.2, we conclude

$$\det J_\varphi = 1 \operatorname{div}(h) + \mathcal{O}(\|h\|^2_{C^1}) \quad \text{and} \quad J_\varphi^{-\top} = I - J_h^\top + \mathcal{O}(\|h\|^2_{C^1}).$$

We use the representation of the divergence operator

$$\operatorname{div}(h) = \operatorname{Div}_{\partial D}(h_\tau) + 2\kappa h_\nu + \frac{\partial h_\nu}{\partial \nu},$$

see [40, Theorem 2.5.20], and compute

$$\frac{\partial h_\nu}{\partial \nu} = \nu^\top J_h \nu + \underbrace{h^\top J_\nu \nu}_{=0} = \nu^\top J_h \nu,$$

since $\mathcal{R} = J_\nu$ acts on the tangential plane, see Lemma 3.11. We consider the Taylor expansion

$$|J_\varphi^{-\top}\nu| = 1 - \nu^\top J_h \nu + \mathcal{O}(\|h\|_{C^1}^2)$$

and arrive at

$$\operatorname{Det}(\varphi) = 1 + \operatorname{Div}_{\partial D} h_\tau + 2\kappa h_\nu + \mathcal{O}(\|h\|_{C^1}^2).$$

The claim follows with the Taylor expansion

$$\widetilde{\lambda} = \lambda + \nabla\lambda^\top h + \mathcal{O}(\|h\|_{C^1}^2).$$

□

Recall κ being the mean curvature, defined in (3.1.20). Now, we are able to prove continuity of the solution with respect to the boundary in the same way as before.

Theorem 3.20. *Let ∂D be of class C^2. If $E \in H_{\mathrm{imp}}(\Omega)$ is the solution of (2.4.8) and $\widehat{E_h} \in H_{\mathrm{imp}}(\Omega)$ a solution of (3.4.3), then we have*

$$\lim_{\|h\|_{C^1}\to 0} \|\widehat{E_h} - E\|_{H_{\mathrm{imp}}(\Omega)} = 0.$$

Proof. Let $B, B_h : H_{\mathrm{imp}}(\Omega) \to H_{\mathrm{imp}}(\Omega)$ be the bounded linear operators, given by the Riesz representation theorem, satisfying

$$\mathcal{B}(E,V) = \langle BE, V\rangle_{H_{\mathrm{imp}}(\Omega)}, \quad \mathcal{B}_h(E,V) = \langle B_h E, V\rangle_{H_{\mathrm{imp}}(\Omega)}$$

for all $E, V \in H_{\mathrm{imp}}(\Omega)$. Then we have

$$\|(B_h - B)E\|_{H_{\mathrm{imp}}(\Omega)}^2 = \mathcal{B}_h(E, (B_h - B)E) - \mathcal{B}(E, (B_h - B)E).$$

By the definition of $\mathcal{B}$ and $\mathcal{B}_h$, the linearizations from Lemma 3.2 and 3.19, together with the Cauchy-Schwarz inequality, we conclude

$$\begin{aligned}
&\|(B_h - B)E\|_{H_{\mathrm{imp}}(\Omega)}^2 \\
&= \int_\Omega \Big[\operatorname{curl} E^\top \Big(\frac{J_\varphi^\top J_\varphi}{\det J_\varphi} - I \Big) \overline{\operatorname{curl}(B_h - B)E} \\
&\qquad\qquad - k^2 E^\top (J_\varphi^{-1} J_\varphi^{-\top} \det J_\varphi - I) \overline{(B_h - B)E} \Big] \,\mathrm{d}x \\
&\quad - \mathrm{i}k \int_{\partial D} \gamma_t E^\top \Big(\widetilde{\lambda} \frac{J_\varphi^\top J_\varphi}{\operatorname{Det}\varphi} - \lambda I \Big) \gamma_t \overline{(B_h - B)E} \,\mathrm{d}s
\end{aligned}$$

$$\leqslant C\|h\|_{C^1}\|E\|_{H_{\mathrm{imp}}(\Omega)}\|(B_h - B)E\|_{H_{\mathrm{imp}}(\Omega)}.$$

We see $B_h \to B$ for $\|h\|_{C^1} \to 0$ and therefore, by a perturbation argument similar to Theorem 3.3, we conclude

$$\|\widehat{E_h} - E\|_{H_{\mathrm{imp}}(\Omega)} \to 0, \quad h \to 0 \text{ in } C^1.$$

□

As before, we continue by proving the existence of the material derivative by taking a closer look at the linearizations from Lemma 3.2 and Lemma 3.19.

Theorem 3.21. *Let ∂D be of class C^2. Let $E \in H_{\mathrm{imp}}(\Omega)$ be the solution of (2.4.8) and $\widehat{E_h} \in H_{\mathrm{imp}}(\Omega)$ of (3.4.3). Then there exists a function $W \in H_{\mathrm{imp}}(\Omega)$, depending linearly and continuously on $h \in C^1$, such that*

$$\lim_{\|h\|_{C^1}\to 0} \frac{1}{\|h\|_{C^1}} \|\widehat{E_h} - E - W\|_{H_{\mathrm{imp}}(\Omega)} = 0.$$

Proof. Similar to the previous cases, we define $W \in H_{\mathrm{imp}}(\Omega)$ as the unique solution of

$$\begin{aligned}
\mathcal{B}(W, V) = &\int_\Omega \operatorname{curl} E^\top \big(\operatorname{div}(h)I - J_h^\top - J_h\big)\overline{\operatorname{curl} V}\,\mathrm{d}x \\
&\qquad + \int_\Omega k^2 E^\top \big(\operatorname{div}(h)I - J_h^\top - J_h\big)\overline{V}\,\mathrm{d}x \\
- \mathrm{i}k &\int_{\partial D} \gamma_t E^\top \Big(\lambda(\operatorname{Div}_{\partial D}(h_\tau) + 2\kappa h_\nu)I - \lambda(J_h + J_h^\top) - (\nabla\lambda^\top h)I\Big)\overline{\gamma_t V}\,\mathrm{d}s
\end{aligned}$$

for all $V \in H_{\mathrm{imp}}(\Omega)$. We have

$$\begin{aligned}
\mathcal{B}(\widehat{E_h} - E - W, V) &= \mathcal{B}(\widehat{E_h}, V) - \ell(V) - \mathcal{B}(W, V) \\
&= \mathcal{B}(\widehat{E_h}, V) - \mathcal{B}_h(\widehat{E_h}, V) - \mathcal{B}(W, V),
\end{aligned}$$

since $\mathcal{B}(E, V) = \ell(V) = \mathcal{B}_h(\widehat{E_h}, V)$ and conclude by considering

$$\begin{aligned}
&\mathcal{B}(\widehat{E_h} - E - W, V) \\
&= \int_\Omega \operatorname{curl} \widehat{E_h}^\top \Big(I - \frac{J_\varphi^\top J_\varphi}{\det J_\varphi} - (\operatorname{div}(h)I - J_h - J_h^\top)\Big)\overline{\operatorname{curl} V}\,\mathrm{d}x \\
&\quad - k^2 \int_\Omega \widehat{E_h}^\top \Big(I - J_\varphi^{-1}J_\varphi^{-\top}\det J_\varphi + (\operatorname{div}(h)I - J_h^\top - J_h)\Big)\overline{V}\,\mathrm{d}x
\end{aligned}$$

$$
\begin{aligned}
&- \mathrm{i}k \int_{\partial D} \gamma_t \widehat{E_h}^\top \Big(\lambda I - \widetilde{\lambda} \frac{J_\varphi^\top J_\varphi}{\operatorname{Det} \varphi} - \lambda(\operatorname{Div}_{\partial D}(h_\tau) + 2\kappa h_\nu) I \\
&\qquad + \lambda(J_h^\top + J_h) + (\nabla \lambda^\top h) I \Big) \overline{\gamma_t V} \, \mathrm{d}s \\
&+ \int_\Omega \operatorname{curl}(\widehat{E_h} - E)^\top (\operatorname{div}(h) I - J_h - J_h^\top) \overline{\operatorname{curl} V} \, \mathrm{d}x \\
&+ k^2 \int_\Omega (\widehat{E_h} - E)^\top (\operatorname{div}(h) I - J_h - J_h^\top) \overline{V} \, \mathrm{d}x \\
&- \mathrm{i}k \int_{\partial D} \gamma_t (\widehat{E_h} - E) \Big(\lambda(\operatorname{Div}_{\partial D}(h_\tau) + 2\kappa h_\nu) I \\
&\qquad - \lambda(J_h + J_h^\top) - (\nabla \lambda^\top h) I \Big) \overline{\gamma_t V} \, \mathrm{d}s,
\end{aligned}
$$

where we added a smart zero and together with the linearizations from Lemmata 3.2 and 3.19

$$
\begin{aligned}
&\frac{1}{\|h\|_{C^1}} \mathcal{B}(\widehat{E_h} - E - W, V) \\
&\qquad \leqslant C \Big(\|\widehat{E_h}\|_{H_{\mathrm{imp}}(\Omega)} \mathcal{O}(\|h\|_{C^1}) + \|\widehat{E_h} - E\|_{H_{\mathrm{imp}}(\Omega)} \Big) \|V\|_{H_{\mathrm{imp}}(\Omega)}
\end{aligned}
$$

for $\|h\|_{C^1} \to 0$. As in Theorem 3.4, we conclude

$$
\lim_{\|h\|_{C^1}} \frac{1}{\|h\|_{C^1}} \|\widehat{E_h} - E - W\|_{H_{\mathrm{imp}}(\Omega)} = 0.
$$

□

Motivated again by the formal Taylor expansion (3.1.6), we can extract the *domain derivative* E' in the same way as for the perfect conductor, see Theorem 3.6.

Theorem 3.22. *Let ∂D be regular. In the setting of Theorem 3.20, we have $E' = W - J_h^\top E - J_E h \in H_{\mathrm{imp}}(\Omega)$. E' can be uniquely extended to the radiating weak solution of Maxwell's equations*

$$
\operatorname{curl} E' - \mathrm{i}k H' = 0, \quad \operatorname{curl} H' + \mathrm{i}k E' = 0
$$

in $\mathbb{R}^3 \setminus \overline{D}$ satisfying the impedance boundary condition

$$
\begin{aligned}
\nu \times H' - \lambda\big(\nu \times (E' \times \nu)\big) &= \overrightarrow{\operatorname{Curl}}_{\partial D}(h_\nu H_\nu) + \lambda \operatorname{Grad}_{\partial D}(E_\nu h_\nu) \\
&+ h_\nu \Big(\frac{\partial \lambda}{\partial \nu} + \mathrm{i}k - 2\lambda(\mathcal{R} - \kappa I) \Big) \big(\nu \times (E \times \nu)\big) + \mathrm{i}k \lambda h_\nu (H \times \nu). \quad (3.4.4)
\end{aligned}
$$

Proof. The proof uses heavily calculations already done in [26], which we also used for the domain derivative of the perfect conductor in Theorem 3.6. First, since the boundary is analytic, we have $E, H \in H^2(\Omega)$, see for example [15, Section 4.5d] and [10, Proposition 2.2]. To be more precise, they show $E, H \in H^s(\Omega)$, if $\partial\Omega$ is of class C^{s+1}. Therefore, we have $\overrightarrow{\operatorname{Curl}}_{\partial D}(h_\nu H_\nu)$ and $\operatorname{Grad}_{\partial D}(h_\nu E_\nu)$ in $L^2_t(\partial D)$, i.e. the right hand side of (3.4.4) is well defined in $L^2_t(\partial D)$. As usual, after defining $E' = W - J_h^\top E - J_E h \in H_{\mathrm{imp}}(\Omega)$, we start by considering

$$\mathcal{B}(E', V) = \mathcal{B}(W, V) - \mathcal{B}(J_h^\top E + J_E h).$$

Since the terms in $\mathcal{B}(W, V)$ involving volume integrals over Ω are exactly the same as in the proof of the characterization of the domain derivative of the perfect conductor, see equation (3.1.10) in the proof of Theorem 3.6, we have

$$\begin{aligned}\mathcal{B}(E', V) = \int_{\partial D} \Big[\operatorname{Grad}_{\partial D}(h^\top \operatorname{curl} E) + k^2(E \times h)\Big]^\top (\nu \times \overline{V})\,\mathrm{d}s \\ - \mathrm{i}k \int_{\partial D} (\nu \times E)^\top \Big[\lambda(\operatorname{Div}_{\partial D}(h_\tau) + 2\kappa h_\nu) I - \lambda(J_h + J_h^\top) - (\nabla\lambda^\top h) I\Big](\nu \times \overline{V})\,\mathrm{d}s \\ + \mathrm{i}k \int_{\partial D} \lambda\big(\nu \times (J_E h + J_h^\top E)\big)^\top (\nu \times \overline{V})\,\mathrm{d}s.\end{aligned}$$

Note, that at this point, we can already conclude that E', together with $H' = \frac{1}{\mathrm{i}k}\operatorname{curl} E'$ is a radiating solution of Maxwell's equations, satisfying some inhomogeneous impedance boundary condition, see (2.4.7), since we have no differential operator applied to the test function $V \in H_{\mathrm{imp}}(\Omega)$. To see, that this function actually is given by (3.4.4), we start to summarize and simplify the terms, using $\nabla\lambda^\top h = h_\nu \frac{\partial\lambda}{\partial\nu} - h_\tau^\top \operatorname{Grad}_{\partial D}\lambda$ and the identity

$$\operatorname{Div}_{\partial D}(h_\tau) + 2\kappa h_\nu = \operatorname{div}(h) - \frac{\partial h_\nu}{\partial \nu},$$

see e.g. [40, Theorem 2.5.20], as well as

$$J_E h + J_h^\top E = \operatorname{curl} E \times h + \nabla(h^\top E),$$

combined with

$$\begin{aligned}\operatorname{curl}(h \times (\nu \times E)) &= h \operatorname{div}(\nu \times E) - (\nu \times E)\operatorname{div}(h) + J_h(\nu \times E) - J_{\nu\times E} h \\ &= h \operatorname{div}(\nu \times E) - (\nu \times E)\operatorname{div}(h) - (J_{\nu\times E} - J_{\nu\times E}^\top) h \\ &\qquad - (J_{\nu\times E}^\top h + J_h^\top(\nu \times E)) + (J_h + J_h^\top)(\nu \times E) \\ &= h \operatorname{div}(\nu \times E) - \operatorname{curl}(\nu \times E) \times h - \nabla(h^\top(\nu \times E))\end{aligned}$$

$$+ (-\operatorname{div}(h)I + J_h + J_h^\top)(\nu \times E)$$

to get

$$\begin{aligned}
&\Big(\lambda(\operatorname{Div}_{\partial D}(h_\tau) + 2\kappa h_\nu)I - \lambda(J_h^\top + J_h) - (\nabla\lambda^\top h)I\Big)(\nu \times E) \\
&= -\frac{\partial \lambda h_\nu}{\partial \nu}(\nu \times E) - h_\tau^\top \operatorname{Grad}_{\partial D}(\lambda)(\nu \times E) - \lambda \operatorname{curl}(h \times (\nu \times E)) \\
&\qquad + \lambda h \operatorname{div}(\nu \times E) - \lambda \operatorname{curl}(\nu \times E) \times h - \lambda \nabla(h^\top(\nu \times E)).
\end{aligned}$$

Note that this calculation requires a smooth extension of ν in a neighborhood of ∂D, which is possible, since ∂D is regular, see [40, Section 2.5.6], where it is shown, that one can choose an extension such that $\operatorname{curl}\nu = 0$ and therefore conclude by (2.2.6)

$$\operatorname{div}(\nu \times E) = E^\top \operatorname{curl}\nu - \nu^\top \operatorname{curl} E = -\nu^\top \operatorname{curl} E = \operatorname{Div}_{\partial D}(\nu \times E)$$

the equivalence of the surface divergence and the regular divergence of $\nu \times E$. Using this, we arrive at

$$\begin{aligned}
\mathcal{B}(E', V) = &\int_{\partial D} \Big[\operatorname{Grad}_{\partial D}(h^\top \operatorname{curl} E) + k^2(E \times h)\Big]^\top (\nu \times \overline{V})\, \mathrm{d}s \\
&+ \mathrm{i}k \int_{\partial D} \lambda(\nu \times (\operatorname{curl} E \times h) + \nu \times \operatorname{Grad}_{\partial D}(h^\top E))^\top (\nu \times \overline{V})\, \mathrm{d}s \\
&- \mathrm{i}k \int_{\partial D} (\nu \times E)^\top \big[-\frac{\partial \lambda h_\nu}{\partial \nu} - h_\tau^\top \operatorname{Grad}_{\partial D} \lambda\big]^\top (\nu \times \overline{V})\, \mathrm{d}s \\
&- \mathrm{i}k \int_{\partial D} \big[\lambda h_\tau \operatorname{Div}_{\partial D}(\nu \times E) - \lambda \operatorname{curl}(\nu \times E) \times h \\
&\qquad - \lambda \operatorname{curl}(h \times (\nu \times E)) - \lambda \operatorname{Grad}_{\partial D}(h^\top(\nu \times E))\big]^\top (\nu \times \overline{V})\, \mathrm{d}s.
\end{aligned}$$

Note, that in every scalar product $F \cdot (\nu \times V)$ for some vector field F, we can drop the normal part or add some normal component, i.e.

$$F \cdot (\nu \times V) = F_\tau \cdot (\nu \times V) = (F + \alpha\nu) \cdot (\nu \times V),$$

where α is an arbitrary scalar function. We gather the terms involving surface gradients as follows:

$$\begin{aligned}
&\operatorname{Grad}_{\partial D}(h^\top \operatorname{curl} E) + \mathrm{i}k(\operatorname{Grad}_{\partial D} \lambda^\top h_\tau)\nu \times E + \mathrm{i}k\lambda \operatorname{Grad}_{\partial D}(h_\tau^\top(\nu \times E)) \\
=&\mathrm{i}k \operatorname{Grad}_{\partial D}(h_\nu H_\nu) + \mathrm{i}k\big(\operatorname{Grad}_{\partial D} \lambda \times (\nu \times E)\big) \times h_\tau,
\end{aligned}$$

where we also used the impedance boundary condition. This leads to

$$\mathcal{B}(E', V) = \int_{\partial D} \Big[\mathrm{i}k \operatorname{Grad}_{\partial D}(h_\nu H_\nu) + \mathrm{i}k\big(\operatorname{Grad}_{\partial D} \lambda \times (\nu \times E)\big) \times h_\tau$$

$$
\begin{aligned}
&\qquad\qquad + k^2(E\times h)\Big]^\top(\nu\times\overline{V})\,\mathrm{d}s\\
&+ \mathrm{i}k\int_{\partial D}\lambda(\nu\times(\operatorname{curl}E\times h)+\nu\times\operatorname{Grad}_{\partial D}(h^\top E))^\top(\nu\times\overline{V})\,\mathrm{d}s\\
&+ \mathrm{i}k\int_{\partial D}\frac{\partial\lambda h_\nu}{\partial\nu}(\nu\times E)^\top(\nu\times\overline{V})\,\mathrm{d}s\\
&- \mathrm{i}k\int_{\partial D}\Big[\lambda h_\tau\operatorname{Div}_{\partial D}(\nu\times E)-\lambda\operatorname{curl}(\nu\times E)\times h\\
&\qquad\qquad - \lambda\operatorname{curl}(h\times(\nu\times E))\Big]^\top(\nu\times\overline{V})\,\mathrm{d}s.
\end{aligned}
$$

Considering $h\times(\nu\times E)=(E^\top h)\nu-h_\nu E$ and again $\operatorname{curl}\nu=0$, we have

$$
\operatorname{curl}(h\times(\nu\times E))=\nabla(h^\top E)\times\nu-\nabla h_\nu\times E-h_\nu\operatorname{curl}E
$$

and therefore

$$
\begin{aligned}
&\mathcal{B}(E',V)\\
&=\int_{\partial D}\Big[\mathrm{i}k\operatorname{Grad}_{\partial D}(h_\nu H_\nu)+\mathrm{i}k\big(\operatorname{Grad}_{\partial D}\lambda\times(\nu\times E)\big)\times h_\tau\\
&\qquad\qquad + k^2(E\times h)\Big]^\top(\nu\times\overline{V})\,\mathrm{d}s\\
&\quad+\mathrm{i}k\int_{\partial D}\Big[\lambda\nu\times(\operatorname{curl}E\times h)+\frac{\partial\lambda h_\nu}{\partial\nu}(\nu\times E)\Big]^\top(\nu\times\overline{V})\,\mathrm{d}s\\
&\quad+\mathrm{i}k\int_{\partial D}\Big[\lambda h_\tau(\operatorname{curl}E)_\nu+\lambda\operatorname{curl}(\nu\times E)\times h\\
&\qquad\qquad - \lambda(\nabla h_\nu\times E)-\lambda h_\nu\operatorname{curl}E\Big]^\top(\nu\times\overline{V})\,\mathrm{d}s.
\end{aligned}
$$

Using $\nu\times(\operatorname{curl}E\times h)=h_\nu\operatorname{curl}E-(\operatorname{curl}E)_\nu h$, we obtain

$$
\begin{aligned}
&\mathcal{B}(E',V)\\
&=\int_{\partial D}\Big[\mathrm{i}k\operatorname{Grad}_{\partial D}(h_\nu H_\nu)+\mathrm{i}k\big(\operatorname{Grad}_{\partial D}\lambda\times(\nu\times E)\big)\times h_\tau+k^2(E\times h)\Big]^\top(\nu\times\overline{V})\,\mathrm{d}s\\
&\quad+\mathrm{i}k\int_{\partial D}\Big[\frac{\partial\lambda h_\nu}{\partial\nu}(\nu\times E)+\lambda\operatorname{curl}(\nu\times E)\times h-\lambda(\nabla h_\nu\times E)\Big]^\top(\nu\times\overline{V})\,\mathrm{d}s.
\end{aligned}
$$

Since we only do need the tangential part of $\nabla h_\nu\times E$, we calculate

$$
(\nabla h_\nu\times E)_\tau=\Big[(\operatorname{Grad}_{\partial D}h_\nu+\frac{\partial h_\nu}{\partial\nu}\nu)\times(E_\nu\nu+E_\tau)\Big]_\tau
$$

$$= E_\nu \operatorname{Grad}_{\partial D} h_\nu \times \nu + \frac{\partial h_\nu}{\partial \nu}(\nu \times E).$$

Recall the curvature operator $\mathcal{R}$ and its properties stated in Lemma 3.11. We use the decomposition of $\operatorname{curl} E$ into tangential and normal component

$$\operatorname{curl} E = (\operatorname{Div}_{\partial D} E \times \nu)\nu + \operatorname{Grad}_{\partial D} E_\nu \times \nu + \Big(\mathcal{R} - 2\kappa - \frac{\partial}{\partial \nu}\Big) E \times \nu,$$

see [40, Theorem 2.5.20], which leads to

$$\operatorname{curl}(\nu \times E) = (\operatorname{Div}_{\partial D} E_\tau)\nu + \Big(\mathcal{R} - 2\kappa - \frac{\partial}{\partial \nu}\Big) E_\tau.$$

Together with the formula

$$\frac{\partial}{\partial \nu} E_\tau - \operatorname{curl} E \times \nu = \operatorname{Grad}_{\partial D} E_\nu - \mathcal{R} E_\tau,$$

see equation (5.4.50) in [40], we arrive at

$$\begin{aligned} \operatorname{curl}(\nu \times E) \times h &= h_\nu \Big[\Big(\mathcal{R} - 2\kappa - \frac{\partial}{\partial \nu}\Big) E_\tau\Big] \times \nu + \operatorname{Div}_{\partial D}(E_\tau)(\nu \times h) \\ = h_\nu \Big[2(\mathcal{R}+\kappa) E_\tau\Big] \times \nu &- \operatorname{Grad}_{\partial D}(E_\nu) \times \nu - \mathrm{i}k h_\nu (H \times \nu) \times \nu + \operatorname{Div}_{\partial D}(E_\tau)(\nu \times h). \end{aligned}$$

It is

$$\big[E_\tau^\top \operatorname{Grad}_{\partial D} \lambda \times h_\tau\big]_\tau = E_\tau^\top \operatorname{Grad}_{\partial D} \lambda (\nu \times h)$$

and therefore with the boundary condition $\nu \times H = \lambda E_\tau$ and with the chain rule for the surface divergence

$$\begin{aligned} \lambda \operatorname{Div}_{\partial D}(E_\tau)(\nu \times h) + (E_\tau^\top \operatorname{Grad}_{\partial D} \lambda)(\nu \times h) &= \operatorname{Div}_{\partial D}(\lambda E_\tau)(\nu \times h) \\ = \operatorname{Div}_{\partial D}(\nu \times H)(\nu \times h) = \mathrm{i}k E_\nu (\nu \times h). \end{aligned}$$

Finally, we have with $\nu \times h_\tau = \nu \times h$

$$\Big[\big(\operatorname{Grad}_{\partial D} \lambda \times (\nu \times E)\big) \times h_\tau\Big]_\tau = (E_\tau^\top \operatorname{Grad}_{\partial D} \lambda)(\nu \times h)$$

and with $\nu \times \nu = 0$ and $(h_\tau \times E_\tau)_\tau = 0$

$$(E \times h)_\tau = E_\nu (\nu \times h) + h_\nu (E \times \nu).$$

If we consider all this, we arrive at

$$\mathcal{B}(E',V) = \mathrm{i}k \int_{\partial D} \Big[\mathrm{Grad}_{\partial D}(h_\nu H_\nu) - \lambda\, \mathrm{Grad}_{\partial D}(h_\nu E_\nu) \times \nu + \frac{\partial \lambda}{\partial \nu}(\nu \times E)$$
$$+ \lambda h_\nu \big[2(\mathcal{R} - \kappa)E_\tau\big] \times \nu - \mathrm{i}k\lambda h_\nu((H \times \nu) \times \nu) - \mathrm{i}k h_\nu (E \times \nu)\Big]^\top (\nu \times \overline{V})\,\mathrm{d}s,$$

or, equivalently,

$$\mathcal{B}(E',V) = \mathrm{i}k \int_{\partial D} \Big[\overrightarrow{\mathrm{Curl}}_{\partial D}(h_\nu H_\nu) + \lambda\, \mathrm{Grad}_{\partial D}(h_\nu E_\nu)$$
$$+ h_\nu \Big(\frac{\partial \lambda}{\partial \nu} + \mathrm{i}k - 2\lambda(\mathcal{R} + \kappa)\Big) E_\tau + \mathrm{i}k\lambda h_\nu (H \times \nu)\Big]^\top (\nu \times (\overline{V} \times \nu))\,\mathrm{d}s.$$

Considering the derivation of the weak formulation (2.4.7), we conclude

$$\nu \times H' - \lambda(\nu \times (E' \times \nu)) = \overrightarrow{\mathrm{Curl}}_{\partial D}(h_\nu H_\nu) + \lambda\, \mathrm{Grad}_{\partial D}(h_\nu E_\nu)$$
$$+ h_\nu \Big(\frac{\partial \lambda}{\partial \nu} + \mathrm{i}k - 2\lambda(\mathcal{R} - \kappa)\Big) E_\tau + \mathrm{i}k\lambda h_\nu^{(} H \times \nu),$$

which finishes the proof. □

Note that again, as expected, the domain derivative E' does only depend on the normal component h_ν of the perturbation on the boundary ∂D, in contrast to the material derivative W, which depends on h in a neighborhood of ∂D.

If one sets $\lambda \equiv \lambda_0 \neq 0$, we arrive at the known characterization of E', see [30, 20]. For non-constant λ, there is also a result on the shape derivative with so-called *generalized impedance boundary condition*, see [10]. Their representation of the shape derivative differs from ours. This is due to the fact, that they use a different way of perturbing the scatterer, where the perturbed scatterer inherits the impedance from the unperturbed scatterer. Recall that we assumed $\lambda \in C^1(\mathbb{R}^3)$ instead, which is more general, since a perturbation h of the scatterer D also changes the corresponding impedance.

The domain derivative does, as expected from the scalar case, see [25], depend on λ in a neighborhood of ∂D, since the characterization involves the normal derivative of λ.

Due to the symmetry of Maxwell's equations, one can conclude from this result the domain derivative for the perfect conductor. Setting $\lambda \equiv 0$, the impedance boundary condition becomes the perfect conducting boundary condition for the magnetic field H. Since (E, H) is a solution of Maxwell's equation if and only if $(H, -E)$ is a solution of Maxwell's equations, we arrive at the boundary condition for E' of the perfect conductor by changing the role of E and H and adding one minus sign, see Theorem 3.6.

4. Inverse scattering problems

Domain derivatives have been used to solve inverse scattering problems. For the acoustic case, see for example [27] for the 2D case and [22] for the 3D case. For the electromagnetic case, see [10] for reconstructions of obstacles with impedance boundary condition.

In this section we want to formulate the inverse problems and the Newton schemes used to solve these. For numerical examples, we refer to Section 6.3. Recall that in each of the settings presented in Section 2.1, i.e. the scattering from a perfect conductor, the scattering from a penetrable obstacle, the scattering from an obstacle with impedance boundary condition or the scattering from an obstacle consisting of chiral media, the bounded scatterer $D \subset \mathbb{R}^3$ is surrounded by an homogeneous medium. In all cases, we imposed the Silver-Müller radiation condition, see (2.1.2) for the scattered field (E^s, H^s). Due to this radiation condition, the scattered field E^s has in the unbounded domain $\mathbb{R}^3 \setminus \overline{D}$ the asymptotic behaviour

$$E^s(x) = \frac{\mathrm{e}^{\mathrm{i}k|x|}}{4\pi|x|}\Big[E_\infty(\hat{x}) + \mathcal{O}\Big(\frac{1}{|x|}\Big)\Big], \quad |x| \to \infty,$$

with $\hat{x} = x/|x|$. E_∞ is called the *electric far field pattern*. It is an analytic tangential vector field on the unit sphere $\mathbb{S}^2$, see [14, Theorem 6.8]. Fixing an incident field (E^i, H^i) and a class of admissible boundaries $\mathcal{Y}$, we can define for each scattering problem the non-linear *(electric) boundary to far field operator*

$$\mathbf{F} : \mathcal{Y} \to L_t^2(\mathbb{S}^2), \quad \partial D \mapsto E_\infty,$$

where E_∞ is the electric far field pattern with respect to the scatterer D with boundary ∂D. The inverse scattering problem then is the following: Given a far field pattern $E_\infty \in L_t^2(\mathbb{S}^2)$, find $\partial D \in \mathcal{Y}$ such that the equation

$$\mathbf{F}(\partial D) = E_\infty \tag{4.0.1}$$

is satisfied. In the light of Section 3, we know $\mathbf{F}$ to be differentiable, i.e. we have

$$\frac{1}{\|h\|_{C^1}}\|\mathbf{F}(\partial D_h) - \mathbf{F}(\partial D) - E'_\infty\|_{L^2(\mathbb{S}^2)} \to 0, \quad h \to 0. \tag{4.0.2}$$

Here E'_∞ denotes the far field pattern of the domain derivative E' with respect the perturbation $h \in C^1(\mathbb{R}^3, \mathbb{R}^3)$ with compact support and with respect to the scatterer $D \subset \mathbb{R}^3$. If we choose a certain type of parametrizations $\mathcal{Y}$ in a subset of a normed space $\mathcal{X}$, (4.0.2) means that the operator $\mathbf{F}$ possesses a Frechét derivative for any admissible boundary ∂D with

$$\mathbf{F}'[\partial D] : \mathcal{X} \to L^2_t(\mathbb{S}^2), \quad \mathbf{F}'[\partial D]h = E'_\infty.$$

Since equation (4.0.1) is ill posed, we use a regularized iterative Newton scheme as follows. First, we choose a starting guess ∂D^0. In every iteration $i \in \mathbb{N}$, we aim to solve

$$\mathbf{F}(\partial D^i_h) = E_\infty \tag{4.0.3}$$

for a variation h. Since this is a non-linear equation we use the linearization

$$\mathbf{F}(\partial D_h) \approx \mathbf{F}(\partial D) + \mathbf{F}'[\partial D]h.$$

Then, (4.0.3) becomes

$$\mathbf{F}'[\partial D^i]h = E_\infty - \mathbf{F}(\partial D^i), \tag{4.0.4}$$

which is now linear in the unknown variation h. We encounter two difficulties. First, (4.0.4) may not be uniquely solvable. Next, due to the ill-posedness of the inverse problem and the unknown non-linear behaviour of $\mathbf{F}$, we have to apply some regularization to damp h, such that the updated scatterer

$$\partial D^{i+1} = \partial D^i_h \tag{4.0.5}$$

is again an admissible boundary. Both difficulties can be contemplated by applying Tikhonov regularization. With some regularization parameter $\alpha > 0$, (4.0.4) becomes then

$$\big(\mathbf{F}'[\partial D^i]^*\mathbf{F}'[\partial D^i] + \alpha\mathbf{I}\big)h = \mathbf{F}'[\partial D^i]^*(E_\infty - \mathbf{F}(\partial D^i)). \tag{4.0.6}$$

After updating $\partial D^{i+1} = \partial D^i_h$, we set $i = i + 1$ and solve again (4.0.6). We stop our iteration, if the residual r_i, defined by

$$r_i = \|\mathbf{F}(\partial D^i) - E_\infty\|_{L^2(\mathbb{S}^2)},$$

falls below a chosen threshold. For more details on such regularized iterative Newton schemes, see [31]. To our knowledge there are no known convergence results for inverse scattering problems.

The implementation of this algorithm requires the computation of $\mathbf{F}$ and $\mathbf{F}'$ as well as its adjoint operator. We will avoid calculating the adjoint of the derivative for our implementation by considering the adjoint of the discretized operator $\mathbf{F}'$. In general, one expects different results if one calculates first the adjoint and discretizes then. In the next section, we want to present the semi-discrete equation which arises from (4.0.6), where $\mathcal{Y}$ and $L^2(\mathbb{S}^2)$ are discretized but the evaluation of $\mathbf{F}$ and $\mathbf{F}'$ for some fixed boundary is not.

4.1. The semi-discrete equation

For now, we are interested in the semi-discrete version of (4.0.6), where we want to discretize $\mathcal{Y}$ but not $\mathbf{F}$ or $\mathbf{F}'$. To ensure that $\mathbf{F}$ possesses a Frechét derivative, we have to choose $\mathcal{Y}$ as an open set of a normed space $\mathcal{X}$. Now let $\mathcal{Y}$ be the set of regular star shaped domains with center in the origin. The boundaries can then be identified by positive smooth functions on the unit sphere $\mathbb{S}^2$ via spherical coordinates, i.e.

$$\mathcal{Y} \ni \partial D = \{x \in \mathbb{R}^3 : x = r(d)\, d, \quad d \in \mathbb{S}^2\}$$

with some smooth function $r : \mathbb{S}^2 \to \mathbb{R}_{>0}$. More precisely, we choose

$$\mathcal{Y} = \{r \in C^\infty(\mathbb{S}^2) : r > 0\}$$

in the normed space $\mathcal{X} = C^\infty(\mathbb{S}^2)$ as domain for the boundary to far field operator $\mathbf{F}$. Recall the definition of the spherical surface harmonics Y_n^m, $n \in \mathbb{N}_0$, $|m| \leqslant n$, which are smooth and form a complete orthonormal system in $L^2(\mathbb{S}^2, \mathbb{C})$, see Lemma 2.7. Any function in this space can be written as a series of spherical surface harmonics. Since we are interested in real-valued functions, we choose for $N \in \mathbb{N}$ the finite dimensional subspace $\mathcal{X}_N \subset \mathcal{X}$, given by

$$\mathcal{X}_N = \{r \in C^\infty(\mathbb{S}^2) : r = \sum_{n=0}^{N} \sum_{m=0}^{n} \alpha_n^m \operatorname{Re} Y_n^m + \sum_{n=1}^{N} \sum_{m=1}^{n} \beta_n^m \operatorname{Im} Y_n^m\},$$

with $\dim(\mathcal{X}_N) = (N+1)^2$, which leads to the discretized set of admissible boundaries $\mathcal{Y}_N$, given by functions $r \in \mathcal{X}_N$ with $r > 0$. Now, we pick $M \in \mathbb{N}$ evaluation points $\hat{x}_1, \dots, \hat{x}_M \in \mathbb{S}^2$ for the evaluation of the far field patterns. Now, $\mathbf{F}(\partial D) = E_\infty$ reads as

$$\mathbf{F}(\alpha, \beta) = (E_\infty(\hat{x}_1), \dots, E_\infty(\hat{x}_M)) \in \mathbb{C}^{3\times M},$$

where $\alpha \in \mathbb{R}^{\frac{(N+1)(N+2)}{2}}$ and $\beta \in \mathbb{R}^{\frac{N(N+1)}{2}}$ denote the vectors of coefficients α_n^m, $n \leqslant N$, $0 \leqslant m \leqslant n$ and β_n^m, $n \leqslant N$, $1 \leqslant m \leqslant n$. Using the linearity of the domain derivative, we can write

$$\mathbf{F}'[\partial D]h = \sum_{n=0}^{N} \sum_{m=0}^{n} \alpha_n^m \mathbf{F}'[\partial D](\operatorname{Re} Y_n^m) + \sum_{n=1}^{N} \sum_{m=1}^{n} \beta_n^m \mathbf{F}'[\partial D](\operatorname{Im} Y_n^m).$$

Again, using only finitely many evaluation points, we have for fixed n and m:

$$\mathbf{F}'[\partial D](\operatorname{Re} Y_n^m) = \big(E'_\infty(\hat{x}_1; \operatorname{Re} Y_n^m), \dots, E'_\infty(\hat{x}_M; \operatorname{Re} Y_n^m)\big) \in \mathbb{C}^{3\times M},$$

$$\mathbf{F}'[\partial D](\operatorname{Im} Y_n^m) = \big(E'_\infty(\hat{x}_1; \operatorname{Re} Y_n^m), \ldots, E'_\infty(\hat{x}_M; \operatorname{Im} Y_n^m)\big) \in \mathbb{C}^{3\times M},$$

where $E'_\infty(\hat{x}; h)$ denotes the far field of the domain derivative E' with respect to the perturbation h, evaluated in $\hat{x} \in \mathbb{S}^2$. Choosing the ordered basis $\mathcal{B}$ of $\mathcal{X}_N$, given by

$$\mathcal{B} = \{\operatorname{Re} Y_0^0, \operatorname{Re} Y_1^0, \operatorname{Re} Y_1^1, \ldots, \operatorname{Re} Y_N^N, \operatorname{Im} Y_1^1, \operatorname{Im} Y_2^1, \ldots, \operatorname{Im} Y_N^N\},$$

we arrive at the representation matrix for the discretized operator $\mathbf{F}'[\partial D]$

$$\begin{aligned}
&\mathbf{F}'[\partial D] : \mathbb{R}^{(N+1)^2} \to \mathbb{C}^{3\times M} \\
&\big(\mathbf{F}'[\partial D]\big)_{ijk} = \big(E'_\infty(\hat{x}_j; h_k)\big)_i, \; i = 1,2,3, \; j = 1, \ldots, M, \; k = 1, \ldots, (N+1)^2,
\end{aligned}$$

where h_k denotes the k-th element of $\mathcal{B}$. As mentioned before, we consider now the adjoint operator of the discretized operator $\mathbf{F}'[\partial D]$, which is just given by transposing and complex conjugation of $\mathbf{F}'[\partial D]$, i.e.

$$\begin{aligned}
\mathbf{F}'[\partial D]^* &: \mathbb{C}^{3\times M} \to \mathbb{R}^{(N+1)^2} \\
\big(\mathbf{F}'[\partial D]^*\big)_{ijk} &= \big(\overline{E'_\infty(\hat{x}_k, h_i)}\big)_j
\end{aligned}$$

with $i = 1, \ldots (N+1)^2$, $j = 1, \ldots, 3$ and $k = 1, \ldots, M$. The product of $\mathbf{F}'[\partial D]^*\mathbf{F}'[\partial D]$ is then given by the complex quadratic $(N+1)^2 \times (N+1)^2$ matrix, given by

$$\big(\mathbf{F}'[\partial D]^*\mathbf{F}'[\partial D]\big)_{ij} = \sum_{k=1}^{M} \overline{E'_\infty(\hat{x}_k; h_i)} \cdot E'_\infty(\hat{x}_k; h_j) \in \mathbb{C}.$$

The discretized version of the identity operator $\mathbf{I}$ in (4.0.6) is just given by the identity matrix $I_{(N+1)^2}$. Instead of $\mathbf{I}$, we choose a different penalty matrix $\mathbf{J}$, which is also a diagonal matrix and the entries are given by $(\mathbf{J})_{kk} = 1 + \lambda(k)$, $k = 1, \ldots, (N+1)^2$. Here, $\lambda(k)$ is the corresponding eigenvalue of the spherical harmonic Y_n^m, associated to the k-th basis element of $\mathcal{B}$, i.e.

$$\lambda(k) := n(n+1), \quad \text{such that } h_k = \operatorname{Re} Y_n^m \text{ or } \operatorname{Im} Y_N^m.$$

This corresponds to an $H^2(\mathbb{S}^2)$-penalty term. The $H^2(\mathbb{S}^2)$-norm is equivalent to the graph norm $\|\cdot\|_{\Delta_{\mathbb{S}^2}}$ of the Laplace-Beltrami Operator $\Delta_{\mathbb{S}^2} : H^2(\mathbb{S}^2) \to L^2(\mathbb{S}^2)$, given by

$$\|\cdot\|_{\Delta_{\mathbb{S}^2}} = \|\cdot\|_{L^2(\mathbb{S}^2)} + \|\Delta_{\mathbb{S}^2} \cdot\|_{L^2(\mathbb{S}^2)},$$

see for example the introduction in [41]. Using an H^2-penalty, which corresponds to the curvature of the boundary, instead of a L^2-penalty is known to improve the results for inverse acoustic scattering problems for star shaped domains, see [25]. We observed similar improvements for inverse electromagnetic scattering problems.

So, solving the Tikhonov equation (4.0.6) after discretization of $\mathcal{Y}$ becomes solving a linear system of $(N+1)^2$ equations. The solution

$$h = (\alpha_h, \beta_h)^\top = (\alpha_0^0, \alpha_1^0, \dots, \alpha_N^N, \beta_1^1, \beta_2^1, \dots, \beta_N^N)^\top \in \mathbb{C}^{(N+1)^2} \tag{4.1.1}$$

of the semi-discrete system

$$\Big(\mathbf{F}'[\partial D]^*\mathbf{F}'[\partial D] + \alpha \mathbf{J}\Big)h = \mathbf{F}'[\partial D]^*\big(E_\infty - \mathbf{F}(\partial D)\big)$$

is in general complex-valued, since both the right hand side and the system matrix are complex-valued. In every iteration, we have to update our boundary, see (4.0.5). After discretization, every boundary ∂D^i is given by a vector of coefficients (α^i, β^i). We update the boundary ∂D^i by discarding the imaginary part of h in (4.1.1). The coefficients of ∂D^{i+1} are then given by

$$(\alpha^{i+1}, \beta^{i+1}) = (\alpha^i + \operatorname{Re}\alpha_h, \beta^i + \operatorname{Re}\beta_h).$$

Full discretization requires additionally the numerical evaluation of $\mathbf{F}(\partial D)$ and $\mathbf{F}'[\partial D]$, which will be addressed in Sections 6.1 and 6.3.

5. Electromagnetic chirality

This section is concerned with so-called electromagnetic chirality, which will be rigorously defined later. It is a phenomenon appearing in electromagnetic scattering, where the scatterer treats incident waves differently according to their helicity. Until recently, the definition of chirality was just a question of geometry. An object is called *(geometrically) achiral*, if it is invariant under some reflection by a plane, combined with translations and rotations and chiral, if that is not the case. This is a purely binary criterium. A scatterer is either chiral or not. In [18], a new definition of electromagnetic chirality was presented, which can also quantify the chiral behaviour. Objects, which are in this sense maximally electromagnetic chiral, are of great interest for applications, since such scatterer are invisible for a certain type of incident fields. In [2], this definition was put into the mathematical context of time-harmonic electromagnetic scattering. Some connections of electromagnetic chirality to geometrical properties were proven and examples presented. We will summarize the main definitions and results in Section 5.1. The author of this thesis was involved in the numerical part of [2], which will be presented in Section 6.2. One of the examples indicates, that the proposed measure of chirality is only continuous and not differentiable and can therefore not be used in a Newton scheme to find scatterers with high measure of chirality. We therefore suggest in Section 5.2 a new measure of chirality and discuss its properties.

5.1. Definition and measurement

All definitions, theorems and proofs in this section are directly from [2]. Recall the Maxwell system in a homogeneous, isotropic material (2.1.1), given by

$$\operatorname{curl} E - \mathrm{i}k\, H = 0, \quad \operatorname{curl} H + \mathrm{i}k\, E = 0. \tag{5.1.1}$$

A simple solution to this system is a plane wave, defined by

$$\begin{pmatrix} E \\ H \end{pmatrix}(x) = \begin{pmatrix} A \\ d \times A \end{pmatrix} \mathrm{e}^{\mathrm{i}k d\cdot x}$$

with amplitude $A \in \mathbb{C}^3$ and direction $d \in \mathbb{S}^2$ with $d \cdot A = 0$. A *Herglotz wave pair* $V[A]$ is a superposition of plane waves with respect to a tangential vector field $A \in L^2_t(\mathbb{S}^2)$, i.e.

$$V[A](x) = \begin{pmatrix} E[A] \\ H[A] \end{pmatrix}(x) = \int_{\mathbb{S}^2} \begin{pmatrix} A(d) \\ d \times A(d) \end{pmatrix} \mathrm{e}^{\mathrm{i}k d\cdot x}\, \mathrm{d}s(d).$$

In general, a solution to the Maxwell system is said to be *left (or right) circularly polarized*, if along a line in the direction of propagation, the real part of the amplitude performs an anticlockwise (or clockwise) circular motion. The amplitude of the electric and magnetic field of a plane wave are always perpendicular. Let $x \in \mathbb{R}^3$ be an observation point. If the amplitudes of the electric and magnetic field perform a circular motion, then the magnetic field at x has to be $+/-$ the electric field if we move one quarter of the wavelength $\lambda = 2\pi/k$ in the direction d of propagation, i.e.

$$\mp(d \times A)\mathrm{e}^{\mathrm{i}kd\cdot x} = \mp H(x) \overset{!}{=} E(x + (\lambda/4)d) = \mathrm{i}A\mathrm{e}^{\mathrm{i}kd\cdot x},$$

i.e. the amplitude satisfies $\mathrm{i}d \times A = \pm A$. Since a Herglotz wave pair is a superposition of plane waves, we have $V[A]$ is left (or right) circularly polarized, if $A \in L^2_t(\mathbb{S}^2)$ is an eigenfunction for the eigenvalue $+1$ (or -1) of the operator

$$\mathcal{C} : L^2_t(\mathbb{S}^2) \to L^2_t(\mathbb{S}), \quad \mathcal{C}A(d) = \mathrm{i}d \times A(d), \quad d \in \mathbb{S}^2.$$

The eigenspaces of $\mathcal{C}$ for the eigenvalues ± 1 are given by

$$V^{\pm} = \{A \pm \mathcal{C}A : A \in L^2_t(\mathbb{S}^2)\}. \tag{5.1.2}$$

These eigenspaces satisfy

$$L^2_t(\mathbb{S}^2) = V^+ \oplus V^-, \quad V^+ \perp V^-$$

with orthogonal projections $\mathcal{P}^{\pm} : L^2_t(\mathbb{S}^2) \to V^{\pm}$, given by $\mathcal{P}^{\pm} = (\mathcal{I} \pm \mathcal{C})/2$. We say a Herglotz wave pair $V[A]$ has *helicity* ± 1 if $A \in V^{\pm}$. So for a Herglotz wave pair, we have an explicit and simple criterium, whether its circularly polarized or not. Since Herglotz wave pairs form a dense set in the space of solutions of the Maxwell system on any compact set, see [12], we only consider these solutions. By the orthogonal decomposition of $L^2_t(\mathbb{S}^2)$ into the eigenspaces $V^{\pm}$ of $\mathcal{C}$, we can decompose any Herglotz wave pair $V[A]$ into a sum of two Herglotz wave pairs, one having helicity $+1$ and the other one having helicity -1. This splitting can be transferred to the solutions: Let $B \subset \mathbb{R}^3$ be a bounded set. If $A \in V^{\pm}$ then $V[A] \in H(\mathrm{curl}, B) \times H(\mathrm{curl}, B)$ satisfies

$$V[A] \in W^{\pm}(B) \times W^{\pm}(B),$$

where the spaces $W^{\pm}(B)$ are given by

$$W^{\pm}(B) = \{U \in H(\mathrm{curl}, B) : \mathrm{curl}\, U = \pm kU\}.$$

Note, that for any solution $(E, H) \in H(\mathrm{curl}, B) \times H(\mathrm{curl}, B)$ of the Maxwell system (5.1.1) the linear combinations

$$E^+ = E + \mathrm{i}H, \quad E^- = E - \mathrm{i}H$$

satisfy $E^\pm \in W^\pm(B)$, i.e. the electric field E admits the decomposition

$$E = \frac{1}{2}(E^+ + E^-)$$

into fields of helicity $+1$ and -1. Let us now consider the following scattering problem: A Herglotz wave pair $V[A]$ is scattered by a bounded scatterer $D \subset \mathbb{R}^3$. This gives rise to a scattered field (E^s, H^s), a solution to the Maxwell system in $\mathbb{R}^3 \setminus \overline{D}$, satisfying the radiation condition (2.1.2). Note that we do not restrict ourselves to one of the special cases presented in Section 2.1, our assumptions hold true for all of them. The far field pattern of a Herglotz wave pair is then given by the *far field operator* $\mathcal{F}$, given by

$$\begin{aligned}
&\mathcal{F} : L^2_t(\mathbb{S}^2) \to L^2_t(\mathbb{S}^2),\\
&\mathcal{F}A(\hat{x}) = \int_{\mathbb{S}^2} E_\infty(\hat{x}, d, A(d))\,\mathrm{d}s(d), \quad \hat{x} \in \mathbb{S}^2.
\end{aligned}$$

Here we used the notion $E_\infty(\hat{x}, d, A)$ for the electric far field pattern E_∞ with respect to an incident plane wave with direction $d \in \mathbb{S}^2$ and amplitude $A \in \mathbb{C}^3$, evaluated in $\hat{x} \in \mathbb{S}^2$. The next theorem states, that the helicity of scattered fields due to incident Herglotz wave pairs can be observed in the far field patterns.

Theorem 5.1. *The far field patterns E_∞, H_∞ are elements of $V^\pm$ if and only if for any bounded open set B such that $\overline{B} \subset \mathbb{R}^3 \setminus \overline{D}$ we have $E^s, H^s \in W^\pm(B)$.*

Proof. See [2, Theorem 2.4]. □

Using the above projections $\mathcal{P}^\pm$, we can decompose the far field operator $\mathcal{F}$ into four operators, i.e.

$$\mathcal{F} = \mathcal{F}^{++} + \mathcal{F}^{+-} + \mathcal{F}^{-+} + \mathcal{F}^{--}$$

with $\mathcal{F}^{pq} = \mathcal{P}^p \mathcal{F} \mathcal{P}^q$ for any pair $p, q \in \{+, -\}$. Each of the projected operators describes the scattering only considering incidents fields of one helicity and scattered fields of one helicity. Now we can finally define the scatterer D to be *electromagnetically achiral*, if there exist unitary operators $\mathcal{U}_j$ in $L^2_t(\mathbb{S}^2)$ with $\mathcal{U}_j \mathcal{C} = -\mathcal{C}\mathcal{U}_j$, $j = 1, \ldots, 4$ such that

$$\mathcal{F}^{++} = \mathcal{U}_1 \mathcal{F}^{--} U_2, \quad \mathcal{F}^{-+} = \mathcal{U}_3 \mathcal{F}^{+-} \mathcal{U}_4$$

holds. If this is not the chase, the scatterer is called *electromagnetically chiral.* Before defining on how to measure how electromagnetically chiral a scatterer is, we first have a look at a geometrical property of a scatterer, which can imply achirality. Recall a scatterer D being called *geometrically achiral*, if there is $x \in \mathbb{R}^3$ and an orthogonal matrix $J \in \mathbb{R}^{3\times 3}$ with $\det J = -1$ such that $D = x + JD$. This means that D is invariant under some reflection by a plane combined with translations and rotations. We have the following theorem.

Theorem 5.2. *If the scatterer D is geometrically achiral and either penetrable or a perfect conductor then D is also electromagnetically achiral.*

Proof. See [2, Theorem 3.2]. $\square$

The context of electromagnetic chirality extends the usual geometric definition. The measure of chirality is motivated by the following observation in [18]: Let (σ_j, x_j, y_j) be a singular system of the electromagnetically achiral far field operator $\mathcal{F}$ and $(\sigma_j^{pq}, x_j^{pq}, y_j^{pq})$ a singular system of $\mathcal{F}^{pq}$ for $p, q \in \{+, -\}$ with decreasing sequences of singular values. Then we have

$$\begin{aligned}\mathcal{F}^{++}\varphi &= \mathcal{U}_1\mathcal{F}^{--}\mathcal{U}_2\varphi = \sum_{j\in\mathbb{N}} \sigma_j^{--}\langle \mathcal{U}_2\varphi, x_j^{--}\rangle \mathcal{U}_1 y_j^{--}\\ &= \sum_{j\in\mathbb{N}} \sigma_j^{--}\langle \varphi, \mathcal{U}_2^* x_j^{--}\rangle \mathcal{U}_1 y_j^{--}\end{aligned}$$

for any $\varphi \in L_t^2(\mathbb{S}^2)$. Therefore, the singular values of $\mathcal{F}^{++}$ and $\mathcal{F}^{--}$ coincide. This is the motivation to define the *measure of chirality* $\chi(\mathcal{F})$ as

$$\chi(\mathcal{F}) = \left(\|(\sigma_j^{++}) - (\sigma_j^{--})\|_{\ell^2}^2 + \|(\sigma_j^{+-}) - (\sigma_j^{-+})\|_{\ell^2}^2\right)^{\frac{1}{2}}.$$

Note that this measure is well defined, since $\mathcal{F}$ is an integral operator with smooth kernel and is therefore known to have at least exponentially decreasing singular values, see [35, Theorem 15.20].

5.2. Smooth measure of chirality

Our first goal is to investigate the regularity of χ. In this section, let c_0 be the space of real-valued sequences with limit 0 and ℓ^2 be space of real-valued square-summable sequences. In the next theorem, we state some well-known results about singular values for the readers convenience.

Theorem 5.3 (Singular system)**.** *Let X, Y be Hilbert spaces and $K, L : X \to Y$ be linear compact operators. Then there exists a sequence $(\mu_j)_{j\in\mathbb{N}}$ and some orthonormal systems $(x_j)_{j\in\mathbb{N}}$ in X and $(y_j)_{j\in\mathbb{N}}$ in Y with*

$$Kx_j = \mu_j y_j, \quad K^* y_j = \mu_j x_j.$$

There is an $x_0 \in \mathcal{N}(K)$ for any $x \in X$ such that we have

$$x = x_0 + \sum_{j\in\mathbb{N}} \langle x, x_j \rangle x_j, \quad Kx = \sum_{j\in\mathbb{N}} \mu_j \langle x, x_j \rangle y_j. \tag{5.2.1}$$

The representation of x is called singular value decomposition. *The non-negative numbers $\mu_j = \mu_j(K)$ are called* singular values. *It is*

$$\lim_{j\to\infty} \mu_j(K) = 0.$$

If we order the singular values such that $\mu_j(K) \geqslant \mu_{j+1}(K)$ holds for every $j \in \mathbb{N}$, we have additionally

$$\mu_1(K) = \|K\|, \quad \mu_{n+1}(K) = \inf_{\psi_1,\dots\psi_n} \sup_{\substack{\varphi\perp\psi_1,\dots,\psi_n \\ \|\varphi\|=1}} \|K\varphi\|, \quad n \in \mathbb{N}.$$

For the singular values of the sum of two compact operators, we have

$$\mu_{n+m+1}(K+L) \leqslant \mu_{n+1}(K) + \mu_{m+1}(L), \quad n, m = 0, 1, 2, \dots. \tag{5.2.2}$$

The triple (μ_j, x_j, y_j) is called singular system of K*.*

Proof. See [35, Theorem 15.16 and 15.17]. □

We define the *singular value decomposition operator* $\mathcal{S}$, which maps a compact operator K onto its sequence of singular values $\mu_j(K)$. A direct consequence of the previous theorem is the following. We denote by $\mathcal{K}(X, Y)$ the space of compact operators from X to Y.

Lemma 5.4. *The singular value decomposition operator*

$$\mathcal{S} : \mathcal{K}(X, Y) \to c_0, \quad K \mapsto (\mu_j(K))_{j\in\mathbb{N}}$$

is Lipschitz continuous.

Proof. Let $K, L \in \mathcal{K}(X, Y)$. Considering (5.2.2) with $n = 0$ we have for $m = 0, 1, 2, \dots$

$$\begin{aligned} \mu_{m+1}(K) = \mu_{m+1}(K - L + L) \leqslant \mu_1(K - L) + \mu_{m+1}(L), \\ \mu_{m+1}(L) = \mu_{m+1}(L - K + K) \leqslant \mu_1(L - K) + \mu_{m+1}(K). \end{aligned}$$

This leads to $\|K - L\| = \mu_1(K - L) \geqslant |\mu_i(L) - \mu_i(K)|$ for all $i \in \mathbb{N}$. Therefore

$$\|\mathcal{S}(K) - \mathcal{S}(L)\|_\infty = \sup_{i\in\mathbb{N}} |\mu_i(K) - \mu_i(L)| \leqslant \mu_1(K - L) = \|K - L\|,$$

i.e. $\mathcal{S}$ is Lipschitz continuous with Lipschitz constant 1. □

Note that $\mathcal{S}$ is not a linear operator, since singular values are always non-negative, i.e. $\mathcal{S}(-K) = \mathcal{S}(K)$ for any compact operator $K \in \mathcal{K}(X,Y)$. As mentioned above, the decrease of the singular values of far field operators is at least exponential, in particular they are elements of ℓ^2. The class of compact operators with square-summable singular values are called *Hilbert Schmidt operators*. We denote the space of Hilbert Schmidt operators between separable Hilbert spaces X and Y with $\mathcal{H}(X,Y)$, which is by means of the next theorem again a Hilbert space.

Theorem 5.5. *Let $(e_j)_j$ be an arbitrary complete orthonormal system in X. We define for $H_1, H_2 \in \mathcal{H}(X,Y)$*

$$\langle H_1, H_2\rangle_{\mathrm{HS}} = \sum_{j\in\mathbb{N}} \langle H_1 e_j, H_2 e_j\rangle_Y .$$

Then $(\mathcal{H}(X,Y), \langle\cdot,\cdot\rangle_{\mathrm{HS}})$ is a Hilbert space. The inner product does not depend on the choice of the orthonormal system $(e_j)_{j\in\mathbb{N}}$. We have

$$\|H\| \leqslant \|H\|_{\mathrm{HS}} = \|\mathcal{S}(H)\|_{\ell^2} = \Big(\sum_{j\in\mathbb{N}} \mu_j^2(H)\Big)^{\frac{1}{2}}$$

for any $H \in \mathcal{H}(X,Y)$.

Proof. See [49, Theorem VI.6.2]. □

Next, we show that $\mathcal{S}$ is continuous from $\mathcal{H}(X,Y)$ to ℓ^2. This is due to the following inequality.

Theorem 5.6 (Von Neumann inequality)**.** *Let $H_1, H_2 \in \mathcal{H}(X,Y)$. Then*

$$|\langle H_1, H_2\rangle_{\mathrm{HS}}| \leqslant \sum_{j\in\mathbb{N}} \mu_j(H_1)\mu_j(H_2) = \langle \mathcal{S}(H_1), \mathcal{S}(H_2)\rangle_{\ell^2} . \tag{5.2.3}$$

Proof. See [19]. □

Now we can prove $\mathcal{S}$ to be again continuous.

Lemma 5.7. *The singular value decomposition operator*

$$\mathcal{S} : \mathcal{H}(X,Y) \to \ell^2, \quad H \mapsto (\mu_j(H))_j$$

is Lipschitz continuous.

Proof. Let $K, L \in \mathcal{H}(X,Y)$. Then we have

$$\begin{aligned}\|\mathcal{S}(K)-\mathcal{S}(L)\|_{\ell^2}^2 &= \sum_{j\in\mathbb{N}} |\mu_j(K)-\mu_j(L)|^2 \\ &= \sum_{j\in\mathbb{N}} \mu_j(K)^2 + \sum_{j\in\mathbb{N}} \mu_j(L)^2 - 2\sum_{j\in\mathbb{N}} \mu_j(K)\mu_j(L).\end{aligned}$$

Note that the first two series converge since $K, L \in \mathcal{H}(X,Y)$ and the last by Cauchy-Schwarz. We apply von Neumann's trace inequality (5.2.3) to the last term to get

$$\operatorname{Re}\langle K, L\rangle_{\mathrm{HS}} \leqslant |\langle K, L\rangle_{\mathrm{HS}}| \leqslant \sum_{j\in\mathbb{N}} \mu_j(K)\mu_j(L)$$

and therefore

$$\|\mathcal{S}(K)-\mathcal{S}(L)\|_{\ell^2}^2 \leqslant \|K\|_{\mathrm{HS}}^2 + \|L\|_{\mathrm{HS}}^2 - 2\operatorname{Re}\langle K, L\rangle_{\mathrm{HS}} = \|K-L\|_{\mathrm{HS}}^2.$$

By taking the root we find $\mathcal{S}$ to be Lipschitz continuous with Lipschitz constant 1. $\square$

The Lipschitz constant 1 is the best we can hope for. This can easily seen by considering for any compact operator K and small $\varepsilon > 0$ the difference

$$\mathcal{S}\big((1+\varepsilon)K\big) - \mathcal{S}(K) = \varepsilon\mathcal{S}(K).$$

We also can not expect $\mathcal{S}$ to be differentiable. Consider Hilbert spaces X and Y with $x \in X$ and $y \in Y$ with $\|x\| = \|y\| = 1$. We define the operators $K, L : X \to Y$ by

$$K = 0, \quad L = \langle\cdot, x\rangle y.$$

They are in particular Hilbert Schmidt operators and we have for $\alpha \neq 0$

$$\frac{1}{\alpha}\Big(\mathcal{S}(K+\alpha L) - \mathcal{S}(K)\Big) = \frac{1}{\alpha}\mathcal{S}(\alpha L) = \frac{|\alpha|}{\alpha}.$$

Since $|\alpha|/\alpha$ does not converge for $\alpha \to 0$, we find $\mathcal{S}$ to be not differentiable in $K = 0$. Let K be an operator with finite dimensional range, which is neither surjective nor injective. This means, there is an $\hat{x} \in X$, $\|\hat{x}\| = 1$ with $K\hat{x} = 0$ and a $\hat{y} \in Y$, $\|\hat{y}\| = 1$ with $\hat{y} \perp K(X)$. Let K be given by the singular value decomposition

$$Kx = \sum_{j=1}^{N} \mu_j \langle x, x_j\rangle y_j$$

for $x \in X$ with $N \in \mathbb{N}$. We define the operator $L : X \to Y$ by

$$Lx = \sum_{j=1}^{N} \mu_j \langle x, x_j \rangle y_j + \frac{\mu_N}{2} \langle x, \hat{x} \rangle \hat{y}.$$

Since the singular values are decreasing, we have for α sufficiently small

$$\frac{1}{\alpha}\Big(\mathcal{S}(K + \alpha L) - \mathcal{S}(K)\Big) = \frac{1}{\alpha}\Big(\alpha\mu_1, \dots, \alpha\mu_N, \frac{|\alpha|\mu_N}{2}\Big),$$

which again does not converge for $\alpha \to 0$. We have shown, that $\mathcal{S} : \mathcal{H}(X,Y) \to \ell^2$ is not differentiable on the set of operators with finite dimensional range, which is dense in $\mathcal{H}(X,Y)$, see [49, Theorem VI.6.2].

We turn our attention again to the measure of chirality χ in the context of Hilbert Schmidt operators. From now on, let X be a separable Hilbert space with two orthogonal subspaces V^+ and V^-, satisfying

$$X = V^+ \oplus^\perp V^-$$

and with orthogonal projections $P^\pm : X \to V^\pm$. Recall the notation $F^{pq} = P^p F P^q$ for any pair $p, q \in \{+, -\}$. Let us abbreviate $\mathcal{H}(X) = \mathcal{H}(X,X)$ and consider the abstract functional

$$\begin{aligned}
&\chi : \mathcal{H}(X) \to \mathbb{R}, \\
&\chi(F) = \sqrt{\|\mathcal{S}(F^{++}) - \mathcal{S}(F^{--})\|_{\ell^2}^2 + \|\mathcal{S}(F^{+-}) - \mathcal{S}(F^{-+})\|_{\ell^2}^2},
\end{aligned}$$

which is of course the measure of chirality, if we set $X = L_t^2(\mathbb{S}^2)$ and consider the spaces $V^\pm$ defined in (5.1.2). Before addressing the regularity of χ, we formulate a Pythagorean theorem for Hilbert Schmidt operators.

Lemma 5.8. *Let $F \in \mathcal{H}(X)$. Then*

$$\|\mathcal{F}\|_{\mathrm{HS}}^2 = \|F^{++}\|_{\mathrm{HS}}^2 + \|F^{-+}\|_{\mathrm{HS}}^2 + \|F^{+-}\|_{\mathrm{HS}}^2 + \|F^{--}\|_{\mathrm{HS}}^2.$$

Proof. Let $F, G \in \mathcal{H}(X)$. We will show

$$\langle F^{pq}, G^{rs} \rangle_{\mathrm{HS}} = \delta_{rp}\delta_{qs} \langle F^{pq}, G^{pq} \rangle_{\mathrm{HS}}$$

for all $p, q, r, s \in \{+, -\}$. Let $(e_j)_{j \in \mathbb{N}}$ be any complete orthonormal system in X. By definition, we have

$$\langle F^{pq}, G^{rs} \rangle_{\mathrm{HS}} = \sum_{j \in \mathbb{N}} \langle F^{qp} e_j, G^{rs} e_j \rangle_X.$$

If $r \neq p$, then we have $F^{pq}e_j \in V^p \perp V^r \ni G^{rs}e_j$ and every summand vanishes. If $s \neq q$, we chose complete orthonormal systems $(u_j)_{j\in\mathbb{N}}$ of V^s and $(v_j)_{j\in\mathbb{N}}$ of V^q. The union of $(u_j)_{j\in\mathbb{N}}$ and $(v_j)_{j\in\mathbb{N}}$ is then a complete orthonormal system of X and we have

$$\begin{aligned}\langle F^{pq}, G^{rs}\rangle_{\mathrm{HS}} &= \sum_{j\in\mathbb{N}} \langle F^{pq}e_j, G^{rs}e_j\rangle_X \\ &= \sum_{j\in\mathbb{N}} \Big(\underbrace{\langle F^{pq}u_j}_{=0}, G^{rs}u_j\rangle_X + \langle F^{pq}v_j, \underbrace{G^{rs}v_j}_{=0}\rangle_X \Big).\end{aligned}$$

The claimed equation follows from $F = F^{++} + F^{+-} + F^{-+} + F^{--}$. □

With this lemma, we immediately conclude, that the measure of chirality $\chi(F)$ is bounded by the Hilbert Schmidt norm $\|F\|_{\mathrm{HS}}$ for any $F \in \mathcal{H}(X)$. In order to investigate higher regularity of χ, one would be interested in the following question: Can one give estimates for the singular values of F^{pq} for $p, q \in \{+,-\}$, if one knows the singular values of F. Unfortunately, a simple example shows, that this is in general not the case. We consider a two dimensional case. Let $x^+, x^- \in X$ with $x^+ \perp x^-$, $\|x^+\|_X = \|x^-\|_X = 1$ and $V^\pm = \operatorname{span}\{x^\pm\}$. The orthogonal projections $P^\pm$ are then given by $P^\pm = \langle \cdot, x^\pm\rangle_X x^\pm$. We define for $\mu > 0$ the linear operators F_1, F_2, given by

$$\begin{aligned} F_1 x &= \frac{\mu}{2}\langle x, x^+ + x^-\rangle_X (x^+ + x^-) \\ F_2 x &= \frac{\mu}{\sqrt{2}}\langle x, (x^+ + x^-)\rangle_X x^+. \end{aligned}$$

Note, that the singular values of F_1 and F_2, coincide, i.e. we have $\mathcal{S}(F_1) = \mathcal{S}(F_2) = \mu$, but we have

$$\mathcal{S}(F_1^{pq}) = \frac{\mu}{2}$$

for all $p, q \in \{+,-\}$ and

$$\mathcal{S}(F_2^{-+}) = \mathcal{S}(F_2^{--}) = 0, \quad \mathcal{S}(F_2^{++}) = \mathcal{S}(F_2^{+-}) = \frac{\mu}{\sqrt{2}}.$$

This means, the singular values of any operator F can be evenly distributed to the projected operators, but it can also happen, that they are concentrated on some of the projected operators. Now we will prove the continuity of the measure of chirality.

Theorem 5.9. *$\chi : \mathcal{H}(X) \to \mathbb{R}$ is continuous.*

Proof. Let $F, F_n \in \mathcal{H}(X)$, $n \in \mathbb{N}$ with $F_n \to F$ in $\mathcal{H}(X)$ as $n \to \infty$. We are using again the fact, that we can choose the complete orthonormal system in the Hilbert Schmidt norm in a convenient way. Let $(x_j)_{j\in\mathbb{N}}$ be a complete orthonormal system of V^q for a fixed $q \in \{+,-\}$, which we complete to a complete orthonormal system of X. Then we have for a fixed $p \in \{+,-\}$

$$\|F^{pq}\|_{\mathrm{HS}}^2 = \sum_{j\in\mathbb{N}} \|P^p F P^q x_j\|^2 \leqslant \sum_{j\in\mathbb{N}} \|P^p F x_j\|^2 \leqslant \sum_{j\in\mathbb{N}} \|F x_j\|^2 = \|F\|_{\mathrm{HS}}^2,$$

since $\|P^p\| = 1$. This means, we have

$$\|F^{pq} - F_n^{pq}\|_{\mathrm{HS}} \leqslant \|F - F_n\|_{\mathrm{HS}} \to 0, \quad n \to \infty.$$

In other words, the mapping $F \mapsto P^p F P^q = F^{pq}$ mapping from $\mathcal{H}(X)$ onto itself is continuous with respect to the Hilbert Schmidt norm. The measure of chirality χ is a composition of continuous mappings, since

$$\chi(F) = \sqrt{\|\mathcal{S}(P^+FP^+) - \mathcal{S}(P^-FP^-)\|_{\ell^2}^2 + \|\mathcal{S}(P^+FP^-) - \mathcal{S}(P^-FP^+)\|_{\ell^2}^2}$$

and therefore continuous. □

As mentioned before, we can not expect differentiability of the measure of chirality χ, since it takes differences of singular values and these singular values do not depend differentiable on the operator with respect to the Hilbert Schmidt norm. First, we make the following observation. Let $F \in \mathcal{H}(X)$. We have $\chi(F) \leqslant \|F\|_{\mathrm{HS}}$ and

$$\begin{aligned}
\chi(F)^2 &= \sum_{j\in\mathbb{N}} \Big(|\mu_j(F^{++}) - \mu_j(F^{--})|^2 + |\mu_j(F^{+-}) - \mu_j(F^{-+})|^2 \Big) \\
&= \sum_{j\in\mathbb{N}} \Big(\mu_j(F^{++})^2 + \mu_j(F^{+-})^2 + \mu_j(F^{-+})^2 + \mu_j(F^{--})^2 \Big) \\
&\qquad - 2\sum_{j\in\mathbb{N}} \Big(\mu_j(F^{++})\mu_j(F^{--}) + \mu_j(F^{+-})\mu_j(F^{-+}) \Big)
\end{aligned}$$

The first series is by Lemma 5.8 just the squared Hilbert Schmidt norm of F, i.e.

$$\chi(F)^2 = \|F\|_{\mathrm{HS}}^2 - 2\sum_{j\in\mathbb{N}} \Big(\mu_j(F^{++})\mu_j(F^{--}) + \mu_j(F^{+-})\mu_j(F^{-+}) \Big). \tag{5.2.4}$$

Since singular values are non-negative and decreasing, we have $\chi(F) = \|F\|_{\mathrm{HS}}$ if and only if either F^{++} or F^{--} and either F^{-+} or F^{+-} vanish. We call such a far field operator *maximally electromagnetically chiral.* In each case the scatterer is invisible with respect to one helicity. Any modification of χ should still have this property. We apply Cauchy Schwarz to (5.2.4). This leads to the *modified measure of chirality* χ_{HS}, given by

$$\begin{aligned}&\chi : \mathcal{H}(X) \to \mathbb{R},\\ &\chi_{\mathrm{HS}}(F) = \sqrt{\|F\|_{\mathrm{HS}}^2 - 2\big(\|F^{++}\|_{\mathrm{HS}}\|F^{--}\|_{\mathrm{HS}} + \|F^{-+}\|_{\mathrm{HS}}\|F^{+-}\|_{\mathrm{HS}}\big)}.\end{aligned}$$

Note, that instead of measuring the difference of every singular value of the corresponding projected operator, we just measure Hilbert Schmidt norms of the projected operators. This will yield higher regularity.

Lemma 5.10. $\chi_{\mathrm{HS}} : \mathcal{H}(X) \to \mathbb{R}$ *is continuous.*

Proof. Let $F \in \mathcal{H}(X)$. Then by Lemma 5.8, we have

$$\|F\|_{\mathrm{HS}}^2 = \|F^{++}\|_{\mathrm{HS}}^2 + \|F^{--}\|_{\mathrm{HS}}^2 + \|F^{+-}\|_{\mathrm{HS}}^2 + \|F^{-+}\|_{\mathrm{HS}}^2.$$

This yields

$$\chi_{\mathrm{HS}}(F) = \sqrt{\big(\|F^{++}\|_{\mathrm{HS}} - \|F^{--}\|_{\mathrm{HS}}\big)^2 + \big(\|F^{+-}\|_{\mathrm{HS}} - \|F^{-+}\|_{\mathrm{HS}}\big)^2}. \tag{5.2.5}$$

Therefore, χ_{HS} is well-defined, since the radicand is non-negative. As seen before, the mapping $F \mapsto P^p F P^q$ is continuous from $\mathcal{H}(X)$ onto itself. This yields, together with the continuity of the Hilbert Schmidt norm $\|\cdot\|_{\mathrm{HS}}$, the result. □

The modified measure of chirality χ_{HS} is bounded and yields the same maximally electromagnetically chiral scatterers as χ.

Lemma 5.11. *We have* $\chi_{\mathrm{HS}}(F) \leqslant \|F\|_{\mathrm{HS}}$ *for any* $F \in \mathcal{H}(X)$*. Let* $F \in \mathcal{H}(X)$ *with* $\|F\|_{\mathrm{HS}} = 1$*. Then*

$$\chi(F) = 1 \Leftrightarrow \chi_{\mathrm{HS}}(F) = 1.$$

Proof. Obviously, $\chi_{\mathrm{HS}}(F)$ is bounded by $\|F\|_{\mathrm{HS}}$ for any $F \in \mathcal{H}(X)$. Let $F \in \mathcal{H}(X)$ with $\|F\|_{\mathrm{HS}} = 1$. As mentioned above, from (5.2.4), we have $\chi(F) = 1$, if and only if one of the following cases holds true:

(i) $F^{++} = 0$ and $F^{+-} = 0$, (ii) $F^{++} = 0$ and $F^{-+} = 0$,

(iii) $F^{--} = 0$ and $F^{+-} = 0$, (iv) $F^{--} = 0$ and $F^{-+} = 0$.

In exactly these cases we have $\chi_{\mathrm{HS}}(F) = 1$, since the non-positive summand $-2(\|F^{++}\|_{\mathrm{HS}}\|F^{--}\|_{\mathrm{HS}} + \|F^{-+}\|_{\mathrm{HS}}\|F^{+-}\|_{\mathrm{HS}})$ vanishes. □

The zeros of the measure of chirality χ are also the zeros of the modified measure of chirality χ_{HS}, as the following Lemma shows.

Lemma 5.12. *Let $F \in \mathcal{H}(X)$. Then*

$$\chi(F) = 0 \Rightarrow \chi_{\mathrm{HS}}(F) = 0.$$

Proof. Let $F \in \mathcal{H}(X)$ with $\chi(F) = 0$. Then $\|F^{++}\|_{\mathrm{HS}} = \|F^{--}\|_{\mathrm{HS}}$ and $\|F^{+-}\|_{\mathrm{HS}} = \|F^{-+}\|_{\mathrm{HS}}$, since the singular values coincide. With (5.2.5), we conclude $\chi_{\mathrm{HS}}(F) = 0$. $\square$

There can be additional zeros of χ_{HS}, as the following example shows. Let $X = \mathbb{R}^3$ and $V^+ = \mathrm{lin}\{e_1, e_2\}$ and $V^- = \mathrm{lin}\{e_3\}$, where e_i denotes for $i = 1, 2, 3$ the i-th standard unit vector. We define the linear operator $F : \mathbb{R}^3 \to \mathbb{R}^3$ by

$$F = \begin{pmatrix} F^{++} & F^{+-} \\ F^{-+} & F^{--} \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ \begin{pmatrix} 0 & 0 \end{pmatrix} & \sqrt{2} \end{pmatrix} \in \mathbb{R}^{3\times 3}.$$

We have $\mu_1(F^{++}) = \mu_2(F^{++}) = 1$ and $\mu_1(F^{--}) = \sqrt{2}$. Additionally, we have $F^{-+} = F^{+-} = 0$. This leads to

$$\chi_{\mathrm{HS}}(F) = \sqrt{\underbrace{\|F\|_{\mathrm{HS}}^2}_{=1+1+2} - 2\big(\underbrace{\|F^{++}\|_{\mathrm{HS}}}_{=\sqrt{2}}\underbrace{\|F^{--}\|_{\mathrm{HS}}}_{=\sqrt{2}} + \underbrace{\|F^{+-}\|_{\mathrm{HS}}\|F^{-+}\|_{\mathrm{HS}}}_{=0}\big)} = 0,$$

but $\chi(F) = \sqrt{(1-\sqrt{2})^2 + 1^2} \neq 0$.

Since even the modified measure of chirality takes the root, we can not expect any higher global regularity than χ_{HS} being continuous. We will therefore consider the squared modified measure of chirality. Even then, it contains the Hilbert Schmidt norm and therefore can not be differentiable. But we can prove χ_{HS}^2 to have some local regularity.

Lemma 5.13. *The squared modified measure of chirality $\chi_{\mathrm{HS}}^2 : \mathcal{H}(X) \to \mathbb{R}$, given by*

$$\chi_{\mathrm{HS}}^2(F) = \|F\|_{\mathrm{HS}}^2 - 2\Big(\|F^{++}\|_{\mathrm{HS}}\|F^{--}\|_{\mathrm{HS}} + \|F^{-+}\|_{\mathrm{HS}}\|F^{+-}\|_{\mathrm{HS}}\Big)$$

is locally Lipschitz.

Proof. Let $p, q \in \{+, -\}$ and $F \in \mathcal{H}(X)$. We consider the continuous function

$$\lambda^{pq}(F) = \|F^{pq}\|_{\mathrm{HS}} = \|P^p F P^q\|_{\mathrm{HS}}.$$

Let additionally $G \in \mathcal{H}(X)$. We have

$$|\lambda^{pq}(F) - \lambda^{pq}(G)| \leqslant \|P^p(F-G)P^q\|_{\mathrm{HS}} \leqslant \|F-G\|_{\mathrm{HS}}.$$

For $p,q,r,s \in \{+,-\}$, we define the product of two of these functionals by

$$\eta_{pq}^{rs}(F) = \lambda^{pq}(F)\lambda^{rs}(F) = \|P^p F P^q\|_{\mathrm{HS}} \|P^r F P^s\|_{\mathrm{HS}}.$$

Then

$$\begin{aligned}
|\eta_{pq}^{rs}(F) - \eta_{pq}^{rs}(G)| &= |\lambda^{pq}(F)\lambda^{rs}(F) - \lambda^{pq}(G)\lambda^{rs}(G)| \\
&= |\lambda^{pq}(F)\lambda^{rs}(F) - \lambda^{pq}(G)\lambda^{rs}(F) + \lambda^{pq}(G)\lambda^{rs}(F) - \lambda^{pq}(G)\lambda^{rs}(F)| \\
&\leqslant \lambda^{rs}(F)|\lambda^{pq}(F) - \lambda^{pq}(G)| + \lambda^{pq}(G)|\lambda^{rs}(F) - \lambda^{rs}(G)| \\
&\leqslant \big(\|F\|_{\mathrm{HS}} + \|G\|_{\mathrm{HS}}\big)\|F-G\|_{\mathrm{HS}}.
\end{aligned}$$

Let now $H \in \mathcal{H}(X)$, $\varepsilon > 0$ and $F, G \in B_\varepsilon(H)$. Then, we define the constant $C_H = 2(\|H\|_{\mathrm{HS}} + \varepsilon)$. From

$$|\eta_{pq}^{rs}(F) - \eta_{pq}^{rs}(G)| \leqslant C_H \|F-G\|_{\mathrm{HS}}$$

we conclude η_{pq}^{rs} to be locally Lipschitz. With

$$\big|\|F\|_{\mathrm{HS}}^2 - \|G\|_{\mathrm{HS}}^2\big| = (\|F\|_{\mathrm{HS}} + \|G\|_{\mathrm{HS}})\big|\|F\|_{\mathrm{HS}} - \|G\|_{\mathrm{HS}}\big| \leqslant C_H \|F-G\|_{\mathrm{HS}}$$

we conclude χ_{HS}^2 to be locally Lipschitz, since it is the sum of locally Lipschitz functions. □

Note that χ_{HS}^2 being locally Lipschitz has strong implications of its regularity in the context of non-smooth analysis and optimization, see for example [11, Chapter 10]. Despite being not necessary differentiable, locally Lipschitz functions admit so called *generalized gradients*, which can be used to identify *descent directions* for non-smooth optimization, see again [11, Chapter 10]. We define the following optimization problem, called *chiral optimization problem*:
Let $f, g : \mathcal{H}(X) \to \mathbb{R}$ defined by

$$\begin{aligned}
f(H) &= 2\big(\|H^{++}\|_{\mathrm{HS}}\|H^{--}\|_{\mathrm{HS}} + \|H^{+-}\|_{\mathrm{HS}}\|H^{-+}\|_{\mathrm{HS}}\big), \\
g(H) &= \|H\|_{\mathrm{HS}}^2 - 1.
\end{aligned}$$

The optimization problem then reads as:

$$\text{Minimize } f(H) \text{ subject to } g(H) = 0$$

on the set of far field operators. Since f is locally Lipschitz, a non-smooth multiplier rule can be applied, see [11, Theorem 10.47]. However, the application of a suitable optimization scheme and the implementation thereof is not part of this thesis. We will finish this chapter with some small results and remarks.

Lemma 5.14. *Let $\mathbb{S} = \{F \in \mathcal{H}(X) : \|F\|_{\mathrm{HS}} = 1\}$. The chiral optimization has infinitely many minimizers $F^* \in \mathbb{S}$. The set of minimizers is path connected.*

Proof. As mentioned above, we have $f(F) = 0$ for $F \in \mathbb{S}$, if and only if one row or one column in the representation matrix of F, given by

$$F = \begin{pmatrix} F^{++} & F^{+-} \\ F^{-+} & F^{--} \end{pmatrix}$$

vanishes. Let $F \in \mathbb{S}$ be a minimizer with $F^{++} \neq 0$ and $F^{+-} = F^{-+} = F^{--} = 0$ and $G \in \mathbb{S}$ be a minimizer with $G^{+-} \neq 0$ and $G^{--} = G^{++} = G^{-+} = 0$. Then $\Gamma : [0,1] \to \mathcal{H}(X)$, given by

$$\Gamma(t) = \begin{pmatrix} \cos(t\pi/2)F^{++} & \sin(t\pi/2)G^{+-} \\ 0 & 0 \end{pmatrix}$$

defines a continuous path with $\Gamma(0) = F$ and $\Gamma(1) = G$. Since the second row vanishes, we have $f(\Gamma(t)) = 0$, i.e. $\Gamma(t)$ is for every $t \in [0,1]$ a minimizer and by Lemma 5.8

$$g(\Gamma(t)) = \cos^2(t\pi/2)\|F\|^2_{\mathrm{HS}} + \sin^2(t\pi/2)\|G\|^2_{\mathrm{HS}} - 1 = 0,$$

i.e. $\Gamma(t) \subset \mathbb{S}$ for $t \in [0,1]$. Similar, if we have $F \in \mathbb{S}$ with vanishing second row, we define the path

$$\Gamma(t) = \begin{pmatrix} F^{++}\sqrt{1 + t\frac{\|F^{+-}\|^2_{\mathrm{HS}}}{\|F^{++}\|^2_{\mathrm{HS}}}} & \sqrt{1-t}F^{+-} \\ 0 & 0 \end{pmatrix}.$$

Then again $g(\Gamma(t)) = 0$ for each $t \in [0,1]$ and $\Gamma(1)$ has only the entry in the upper left corner. Two operators F, G with only one entry can be transformed into each other via a rotation in the plane by the angle α defined by $\cos(\alpha) = \langle F, G\rangle_{\mathrm{HS}}$. With these prototype paths we can construct now paths from any minimizer to another. $\square$

We want to emphasize at this point that this Lemma does not state, that there is a scatterer D, such that its associated far field operator F satisfies

$\chi(F) = \|F\|_{\mathrm{HS}}$. If we restrict ourselves to one scattering problem and a certain type of geometries, it is still not clear, how the set of far field operators does look like. Since the function f from the chiral optimization involves norms, it is differentiable, whenever none of these norms vanish.

Lemma 5.15. *Let $\mathcal{O} = \{F \in \mathcal{H}(X) : F^{pq} \neq 0 \text{ for all } p, q \in \{+,-\}\}$. Then $f : \mathcal{O} \to \mathbb{R}$ is differentiable with*

$$f'[F]G = 2\left(\frac{\|F^{--}\|_{\mathrm{HS}}}{\|F^{++}\|_{\mathrm{HS}}} \operatorname{Re}\langle F^{++}, G^{++}\rangle_{\mathrm{HS}} + \frac{\|F^{++}\|_{\mathrm{HS}}}{\|F^{--}\|_{\mathrm{HS}}} \operatorname{Re}\langle F^{--}, G^{--}\rangle_{\mathrm{HS}}\right.$$
$$\left. + \frac{\|F^{+-}\|_{\mathrm{HS}}}{\|F^{-+}\|_{\mathrm{HS}}} \operatorname{Re}\langle F^{-+}, G^{-+}\rangle_{\mathrm{HS}} + \frac{\|F^{-+}\|_{\mathrm{HS}}}{\|F^{+-}\|_{\mathrm{HS}}} \operatorname{Re}\langle F^{+-}, G^{+-}\rangle_{\mathrm{HS}}\right)$$

for $F \in \mathcal{O}$ and $G \in \mathcal{H}(X)$.

Proof. For any $p, q \in \{+,-\}$, we consider $\lambda^{pq}(F) = \langle P^p F P^q, P^p F P^q\rangle_{\mathrm{HS}}$. Then we have for $F, G \in \mathcal{H}(X)$

$$\lambda^{pq}(F + tG) - \lambda^{pq}(F) = 2t \operatorname{Re}\langle P^p F P^q, P^p G P^q\rangle_{\mathrm{HS}} + t^2\langle P^p G P^q, P^p G P^q\rangle_{\mathrm{HS}}.$$

We conclude $(\lambda^{pq})'[F]G = 2 \operatorname{Re}\langle F^{pq}, G^{pq}\rangle_{\mathrm{HS}}$. The claim follows by the product and chain rule. $\square$

The literature is not consistent on how to define *directional derivatives.* Following [11], a directional derivative $F'(x; y)$ of a mapping $F : X \to Y$ between normed spaces X and Y at a point $x \in X$ in direction $y \in X$ is, if it exists, the following limit:

$$F'(x; y) = \lim_{t \to 0+} \frac{F(x + ty) - F(x)}{t}.$$

Note that some authors, see [29, 48], require $t \to 0$ in the limit. Then, less functions possess a directional derivative. By the above definition, we conclude by

$$\lim_{t \to 0+} \frac{1}{t}\big(\|(F + tG)^{pq}\|_{\mathrm{HS}} - \|F^{pq}\|_{\mathrm{HS}}\big) = \|G^{pq}\|_{\mathrm{HS}}$$

that the function f from the chiral optimization admits in every point the directional derivative in every direction.

Finally, we observe that f has no local minimizers on $\mathcal{O}$.

Lemma 5.16. *We have $f'[F] \neq 0$ for every $F \in \mathcal{O}$.*

Proof. Assume $f'[F] = 0$ for some $F \in \mathcal{O}$. Then choosing $G = F^{++}$ and considering Lemma 5.8, we conclude

$$0 = f'[F]F^{++} = \frac{\|F^{--}\|_{\mathrm{HS}}}{\|F^{++}\|_{\mathrm{HS}}} \operatorname{Re}\langle F^{++}, F^{++}\rangle_{\mathrm{HS}} = \|F^{--}\|_{\mathrm{HS}} \|F^{++}\|_{\mathrm{HS}}.$$

So either $F^{++} = 0$ or $F^{--} = 0$, a contradiction. $\square$

6. Numerical examples

In this section, we present numerical examples illustrating the previous sections. The common theme of Section 4 and 5 is that we have to solve electromagnetic scattering problems. In Section 4, we have to calculate the solution (E, H) of the scattering problem numerically, as well as the domain derivative E'. Since the domain derivative E' is again a solution of the same scattering problem as (E, H), the same techniques can be used. But the boundary condition of the domain derivative contains the solution (E, H) of the scattering problem, see Theorems 3.6, 3.13 and 3.22 and involves surface differential operators as well as curvature terms. In Section 5, we have to calculate a discretization of the far field operator $\mathcal{F}$. This means, we have to choose a convenient basis of $L^2_t(\mathbb{S}^2)$ and calculate the far field for many elements of this basis. In Section 2.4, we presented the weak formulations of the scattering from a perfect conductor and from an obstacle with impedance boundary condition. So one could naturally choose a finite element approach in order to solve these equations, see [39]. We chose a boundary integral equations approach. Looking closely at the boundary conditions of the domain derivatives, we identify the traces of the solutions (E, H) and terms with surface differential operators applied to the solution. Therefore an integral equation approach, where these traces are the unknowns seems reasonable. On the other hand we avoid having a three-dimensional computational region, which changes at every iteration of the Newton scheme. Lastly, at the beginning of this work, there was to the best of our knowledge no open source finite element library available, which satisfied all of our needs. The actual implementations are carried out in the open source Galerkin boundary element methods library BEMPP (`https://bempp.com/`). For an overview of the library, see [47]. We start by presenting the derivation of boundary integral equations for the considered scattering problems. See [50, Section 3.3] for an overview of such equations and for more details we refer to [7, 8].

6.1. Integral equations of scattering problems

We consider the Maxwell system

$$\operatorname{curl} E = \mathrm{i}k\, H, \quad \operatorname{curl} H = -\mathrm{i}k\, E$$

with wavenumber $k \in \mathbb{R}$ in some region Ω with boundary $\partial\Omega$. We start this section with the famous *Stratton-Chu representation formula.* In order to do this, we define the *magnetic* or *Neumann-trace*

$$\gamma_N : H(\operatorname{curl}^2, \Omega) \to H^{-\frac{1}{2}}(\operatorname{Div}, \partial\Omega),$$

$$\gamma_N \varphi = \frac{1}{\mathrm{i}k} \operatorname{curl} \varphi \times \nu.$$

The term magnetic comes from the fact, that if $(\varphi, \frac{1}{\mathrm{i}k} \operatorname{curl} \varphi)$ is a solution of the Maxwell system, then $\gamma_N \varphi$ is the trace of the magnetic field. By Theorem 2.5, we have that γ_N is continuous. Let Φ denote the *fundamental solution* of the three-dimensional Helmholtz equation $\Delta u + k^2 u = 0$, i.e.

$$\Phi(x, y) = \frac{1}{4\pi} \frac{\mathrm{e}^{\mathrm{i}k|x-y|}}{|x-y|}.$$

Then we define the *electric potential*

$$\mathcal{E}\varphi(x) = \mathrm{i}k \int_{\partial\Omega} \varphi(x)\Phi(x, y) \, \mathrm{d}s(y) - \frac{1}{\mathrm{i}k} \nabla \int_{\partial\Omega} \operatorname{Div}_{\partial\Omega} \varphi(y)\Phi(x, y) \, \mathrm{d}s(y),$$

as well as the *magnetic potential*

$$\mathcal{H}\varphi(x) = \operatorname{curl} \int_{\partial\Omega} \varphi(y)\Phi(x, y) \, \mathrm{d}s(y).$$

We want to motivate the names electric and magnetic potential. Let φ be a smooth tangential vector field. We define $E = \mathcal{E}\varphi$. Then

$$\operatorname{curl} E(x) = \mathrm{i}k \operatorname{curl} \int_{\partial\Omega} \varphi(x)\Phi(x, y) \, \mathrm{d}s(y) = \mathrm{i}k \, \mathcal{H}\varphi(x).$$

On the other hand, if we define $H = \mathcal{H}\varphi$, we have

$$\begin{aligned}
\operatorname{curl} H(x) &= \operatorname{curl} \operatorname{curl} \int_{\partial\Omega} \varphi(y)\Phi(x, y) \, \mathrm{d}s(y) \\
&= (\nabla \operatorname{div} - \Delta) \int_{\partial\Omega} \varphi(y)\Phi(x, y) \, \mathrm{d}s(y) \\
&= k^2 \int_{\partial\Omega} \varphi(y)\Phi(x, y) \, \mathrm{d}s(y) + \nabla \int_{\partial\Omega} \operatorname{div}_x \big(\varphi(y)\Phi(x, y)\big) \, \mathrm{d}s(y) \\
&= k^2 \int_{\partial\Omega} \varphi(y)\Phi(x, y) \, \mathrm{d}s(y) + \nabla \int_{\partial\Omega} \varphi(y) \cdot \nabla_x \Phi(x, y) \, \mathrm{d}s(y) \\
&= k^2 \int_{\partial\Omega} \varphi\Phi(x, y) \, \mathrm{d}s(y) - \nabla \int_{\partial\Omega} \varphi(y) \nabla_y \Phi(x, y) \, \mathrm{d}s(y).
\end{aligned}$$

Since φ is a tangential vector field, the integrand of the second integral becomes $\varphi(y) \cdot \operatorname{Grad}_{\partial\Omega} \Phi(x, y)$. We apply the partial integration formula for the surface gradient (2.2.5) and arrive at

$$\operatorname{curl} H(x) = -\mathrm{i}k \, \mathcal{E}\varphi(x) = -\mathrm{i}k \, E(x).$$

In other words: For any $\varphi \in C_t^1(\partial\Omega, \mathbb{C}^3)$, the pair $(\mathcal{E}\varphi, \mathcal{H}\varphi)$ forms a solution to the Maxwell system.

In order to state the continuity result for these potentials, we need to define additional function spaces. Let $L^2_{\text{loc}}(\Omega)$ be the *space of locally square integrable functions*, i.e. $E \in L^2_{\text{loc}}(\Omega)$ if and only if $E \in L^2(\widetilde{\Omega})$ for any bounded set $\widetilde{\Omega} \subset \Omega$. Of course, if Ω is bounded itself, we have $L^2_{\text{loc}}(\Omega) = L^2(\Omega)$. Similarly we define the spaces of locally square integrable $H(\text{curl}, \Omega)$ functions

$$H_{\text{loc}}(\text{curl}, \Omega) = \{E \in L^2_{\text{loc}}(\Omega) : \text{curl}\, E \in L^2_{\text{loc}}(\Omega)\}.$$

Finally, we define the space of functions $E \in L^2(\Omega, \mathbb{C}^3)$ which posses weak $\text{curl}\,\text{curl}\, E \in L^2(\Omega, \mathbb{C}^3)$ and the space of those functions which are additionally square integrable by

$$\begin{aligned} H(\text{curl}^2, \Omega) &= \{E \in H(\text{curl}, \Omega) : \text{curl}\,\text{curl}\, E \in L^2(\Omega, \mathbb{C}^3)\}, \\ H_{\text{loc}}(\text{curl}^2, \Omega) &= \{E \in H_{\text{loc}}(\text{curl}, \Omega) : \text{curl}\,\text{curl}\, E \in L^2_{\text{loc}}(\Omega, \mathbb{C}^3)\}. \end{aligned}$$

Theorem 6.1. *The electric and magnetic potential are continuous as mappings from $H^{-\frac{1}{2}}(\text{Div}, \partial\Omega)$ to $H_{\text{loc}}(\text{curl}^2, \Omega)$.*

Proof. See [7, Theorem 5]. □

With these definitions, we can now state the *Stratton-Chu representation formula*, which motivates in hindsight the definition of the electric and magnetic potentials.

Theorem 6.2 (Stratton-Chu)**.** *Let $E \in H_{\text{loc}}(\text{curl}^2, \Omega)$ be a solution of the Maxwell system in Ω. If Ω is bounded, then we have*

$$E = \mathcal{H}\gamma_t E + \mathcal{E}\gamma_N E \quad \textit{in } H(\text{curl}^2, \Omega).$$

If Ω is the exterior of some bounded domain and E satisfies additionally the Silver-Müller radiation condition, then

$$E = -\mathcal{H}\gamma_t E - \mathcal{E}\gamma_N E \quad \textit{in } H_{\text{loc}}(\text{curl}^2, \Omega).$$

Proof. See [7, Theorem 6]. □

For the moment, we assume that Ω is a bounded domain with boundary $\partial\Omega$. For $\varphi \in H_{\text{loc}}(\text{curl}^2, \Omega \bigcup \mathbb{R}^n \setminus \overline{\Omega})$ we denote by γ_t^-, γ_N^- the interior traces, i.e.

$$\gamma_t^- \varphi = \gamma_t\big(\varphi\big|_\Omega\big) \in H^{-\frac{1}{2}}(\text{Div}, \partial\Omega), \quad \gamma_N^- \varphi = \gamma_N\big(\varphi\big|_\Omega\big) \in H^{-\frac{1}{2}}(\text{Div}, \partial\Omega)$$

and by γ_t^+, γ_N^+ the exterior traces. We introduce the notation

$$[\gamma\varphi]_\pm = \gamma^+\varphi - \gamma^-\varphi$$

for the jump of some trace γ on the boundary $\partial\Omega$ and the notation

$$\{\gamma\varphi\}_\pm = \frac{1}{2}(\gamma^+\varphi + \gamma^-\varphi)$$

for the mean of some trace γ. The potentials map $H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega)$ onto the space $H_{\mathrm{loc}}(\mathrm{curl}^2, \Omega \bigcup \mathbb{R}^3 \setminus \overline{\Omega})$. We can therefore take interior and exterior traces of the potentials. These traces satisfy the following jump relations.

Theorem 6.3. *We have*

$$[\gamma_t \mathcal{E}\varphi]_\pm = [\gamma_N \mathcal{H}\varphi]_\pm = 0 \quad \text{and} \quad [\gamma_N \mathcal{E}\varphi] = [\gamma_t \mathcal{H}\varphi]_\pm = -\varphi$$

for $\varphi \in H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega)$.

Proof. See [7, Theorem 7]. □

We use the traces of the electric and magnetic potentials to define the *electric boundary operator* **E** by taking the mean of the tangential traces, i.e.

$$\begin{aligned} &\mathbf{E} : H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega) \to H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega), \\ &\varphi \mapsto \{\gamma_t \mathcal{E}\varphi\}_\pm \end{aligned}$$

and analogously the *magnetic boundary operator* **H** by

$$\begin{aligned} &\mathbf{H} : H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega) \to H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega), \\ &\varphi \mapsto \{\gamma_t \mathcal{H}\varphi\}_\pm. \end{aligned}$$

The interior and exterior traces of the potentials and the boundary operators are coupled in the following way.

Lemma 6.4. *We have*

$$\begin{aligned} \gamma_t^\pm \mathcal{E} &= \mathbf{E}, & \gamma_N^\pm \mathcal{E} &= \mp\frac{1}{2}\mathbf{I} + \mathbf{H}, \\ \gamma_t^\pm \mathcal{H} &= \mp\frac{1}{2}\mathbf{I} + \mathbf{H}, & \gamma_N^\pm \mathcal{H} &= -\mathbf{E}. \end{aligned}$$

Proof. These relations follow from the jump relations in Theorem 6.3 and from

$$\{\gamma_N \mathcal{E}\}_\pm = \mathbf{H}, \quad \{\gamma_N \mathcal{H}\}_\pm = -\mathbf{E}. \tag{6.1.1}$$

From the calculations shown in the motivation on naming the potentials, we conclude by a density argument

$$\gamma_N \mathcal{E} = \gamma_t \mathcal{H}, \quad \gamma_N \mathcal{H} = -\gamma_t \mathcal{E},$$

which shows (6.1.1). $\square$

We define the *multitrace operator* $\mathbf{A}$ by

$$\mathbf{A} = \begin{pmatrix} \mathbf{H} & \mathbf{E} \\ -\mathbf{E} & \mathbf{H} \end{pmatrix}.$$

With the multitrace operator, we finally define the *exterior* and *interior Calderón projector*

$$\mathbf{C}^{\pm} : H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega)^2 \to H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega)^2$$

by the matrix

$$\mathbf{C}^{\pm} = \frac{1}{2}\mathbf{I} \mp \mathbf{A} = \begin{pmatrix} \frac{1}{2}\mathbf{I} \mp \mathbf{H} & \mp\mathbf{E} \\ \pm\mathbf{E} & \frac{1}{2}\mathbf{I} \mp \mathbf{H} \end{pmatrix}.$$

All the above potentials and operators depend on the corresponding wavenumber. Considering penetrable objects with interior and exterior wavenumber k and κ, we will denote the dependency for example by $\mathcal{E}_k$ and $\mathcal{E}_\kappa$ for the electric potential with respect to the interior and exterior wavenumber. In the context of the perfect conductor and the scattering from an obstacle with impedance boundary condition where only one wavenumber occurs, we will just write $\mathcal{E}$ for the electric potential. The traces of solutions of the Maxwell system are exactly eigenfunctions of the Calderón projector.

Theorem 6.5. *Let Ω be a bounded domain and $E \in H_{\mathrm{loc}}(\mathrm{curl}^2, \Omega \bigcup \mathbb{R}^3 \setminus \overline{\Omega})$ be a solution of the Maxwell system in Ω and $\mathbb{R}^3 \setminus \Omega$ and also satisfying the Silver-Müller radiation condition. Then we have*

$$\mathbf{C}^{\pm} \begin{pmatrix} \gamma_t^{\pm} E \\ \gamma_N^{\pm} E \end{pmatrix} = \begin{pmatrix} \gamma_t^{\pm} E \\ \gamma_N^{\pm} E \end{pmatrix}. \tag{6.1.2}$$

On the other hand, any pair $a, b \in H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega)$ with $\mathbf{C}^p(a,b)^\top = (a,b)^\top$ for $p \in \{+,-\}$ can be identified as the traces of a solution $E \in H(\mathrm{curl}^2, \Omega)$ if $p = -$ and $E \in H(\mathrm{curl}^2, \mathbb{R}^3 \setminus \overline{\Omega})$ if $p = +$ of the Maxwell system, i.e. $a = \gamma_t^p E$ and $b = \gamma_N^p E$. In the exterior case, E satisfies the Silver-Müller radiation condition.

Proof. Let $E \in H_{\mathrm{loc}}(\mathrm{curl}^2, \Omega \bigcup \mathbb{R}^3 \setminus \overline{\Omega})$ be a solution of the Maxwell system in Ω and $\mathbb{R}^3 \setminus \overline{\Omega}$, satisfying the radiation condition. By Stratton-Chu, we have

$$E = \mathcal{H}\gamma_t^- E + \mathcal{E}\gamma_N^+ E \quad \text{in } H(\mathrm{curl}^2, \Omega)$$

and

$$E = -\mathcal{H}\gamma_t^+ E - \mathcal{H}\gamma_N^- E \quad \text{in } H_{\mathrm{loc}}(\mathrm{curl}^2, \mathbb{R}^3 \setminus \overline{\Omega}).$$

Taking the exterior and interior tangential trace $\gamma_t^\pm$ of the corresponding equation and considering the jump relations from Lemma 6.4, we arrive at the first equation of (6.1.2). Taking the exterior and interior magnetic trace $\gamma_N^\pm$ yields the second one. Let now the pair $a, b \in H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega)$ satisfy $\mathbf{C}^-(a,b)^\top = (a,b)^\top$. We define a vector field $E \in H(\mathrm{curl}^2, \Omega)$ by

$$E = \mathcal{H}a + \mathcal{E}b$$

and set $H = \frac{1}{\mathrm{i}k} \mathrm{curl}\, E$. Then (E, H) is a solution of the Maxwell system in Ω with

$$\gamma_t^- E = \gamma_t^- \mathcal{H}a + \gamma_t^- \mathcal{E}b = \Big(\frac{1}{2}\mathbf{I} + \mathbf{H}\Big)a + \mathbf{E}b = a,$$
$$\gamma_N^- E = \gamma_N^- \mathcal{H}a + \gamma_N^- \mathcal{E}b = -\mathbf{E}a + \Big(\frac{1}{2}\mathbf{I} + \mathbf{H}\Big)b = b,$$

since these are just the two equations of $\mathbf{C}^-(a,b)^\top = (a,b)^\top$. One can argue similarly for the exterior case. □

6.1.1. Perfect conductor

Let D be a bounded Lipschitz domain and $k \in \mathbb{R}$. Recall the scattering problem for the perfect conductor, which reads as

$$\mathrm{curl}\, E^s = \mathrm{i}k\, H^s, \quad \mathrm{curl}\, H^s = -\mathrm{i}k\, E^s \quad \text{in } \mathbb{R}^3 \setminus \overline{D}, \tag{6.1.3a}$$
$$\nu \times E^s + \nu \times E^i = 0, \quad \text{on } \partial D, \tag{6.1.3b}$$
$$\lim_{|x|\to\infty} |x| \big[H^s(x) \times \frac{x}{|x|} - E^s(x)\big] = 0, \tag{6.1.3c}$$

where the pair (E^i, H^i) is a solution of (6.1.3a) in $\mathbb{R}^3$. To get an integral equation, there are in general two established approaches. The first one, called *indirect*, starts by making an Ansatz, for example

$$E^s(x) = -\mathcal{E}\lambda(x), \quad x \in \mathbb{R}^3 \setminus \overline{D}$$

for some to be determined $\lambda \in H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega)$. Then, one applies the trace and injects the boundary condition (6.1.3b), which yields the so called *indirect electric field integral equation (EFIE)*, given by

$$\mathbf{E}\lambda = \gamma_t E^i. \tag{6.1.4}$$

Note that in contrast to the exterior problem (6.1.3a) - (6.1.3c), the indirect EFIE (6.1.4) is not always uniquely solvable. Unique solvability depends on whether k is a so called *interior eigenvalue* of D, see [7, Definition 4]. From now on, we will always assume, that that is not the case. This is not a strong assumption, since these critical values of k form a discrete sequence accumulating at infinity. Of course, we can also choose the magnetic potential in our Ansatz, i.e.

$$E^s(x) = \mathcal{H}\lambda(x), \quad x \in \mathbb{R}^3 \setminus \overline{D},$$

which leads to the so called *indirect magnetic field integral equation (MFIE)*, given by

$$\Big(\frac{1}{2}\mathbf{I} + \mathbf{H}\Big)\lambda = \gamma_t E^i. \tag{6.1.5}$$

Recall $(\gamma_t^+ E^s, \gamma_N^+ E^s)$ being an eigenfunction of the Calderón projector $\mathbf{C}^+$. The direct approach starts by considering the first equation of

$$\mathbf{C}^+ \begin{pmatrix} \gamma_t^+ E^s \\ \gamma_N^+ E^s \end{pmatrix} = \begin{pmatrix} \gamma_t^+ E^s \\ \gamma_N^+ E^s \end{pmatrix}. \tag{6.1.6}$$

By the boundary condition, only $\gamma_N^+ E^s$ is unknown. This leads to *direct electric field integral equation (EFIE)*, given by

$$\mathbf{E}\lambda = \Big(\frac{1}{2}\mathbf{I} + \mathbf{H}\Big)\gamma_t^+ E^i \tag{6.1.7}$$

for the unknown Neumann trace $\lambda = \gamma_N^+ E^s \in H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega)$. Finally, considering the second equation of (6.1.6), we arrive at the *direct magnetic field integral equation (MFIE)*, given by

$$\Big(\frac{1}{2}\mathbf{I} + \mathbf{H}\Big)\lambda = -\mathbf{E}\gamma_t^+ E^i \tag{6.1.8}$$

for the unknown Neumann trace $\lambda = \gamma_N^+ E^s \in H^{-\frac{1}{2}}(\mathrm{Div}, \partial\Omega)$. Considering calculation time, the indirect approach profits from a *cheap* right hand side, since only the magnetic or the electric boundary integral operator have to be assembled. On the other hand, if one is interested in the magnetic trace $\gamma_N^+ E^s$, for example to calculate the boundary condition of the domain derivative, see (3.1.7), then the direct approach profits from the fact, that the unknown λ is exactly the magnetic trace $\gamma_N^+ E^s$.

6.1.2. Penetrable Obstacles

Let again $D \subset \mathbb{R}^3$ be a bounded Lipschitz domain. Recall the scattering from a penetrable obstacle: Let $\kappa > 0$ denote the interior and $k > 0$ the exterior wavenumber. Furthermore, we have the interior material coefficients $\mu_D, \varepsilon_D > 0$ and the exterior material coefficients $\mu_0, \varepsilon_0 > 0$, see Section 2.1.2. Then the full scattering problem reads as:

$$\operatorname{curl} E = \mathrm{i}\kappa\, H, \quad \operatorname{curl} H = -\mathrm{i}\kappa\, E \quad \text{in} D, \tag{6.1.9a}$$

$$\operatorname{curl} E = \mathrm{i}k\, H, \quad \operatorname{curl} H = -\mathrm{i}k\, E \quad \text{in } \mathbb{R}^3 \setminus \overline{D}, \tag{6.1.9b}$$

$$\frac{1}{\sqrt{\varepsilon_0}} \nu \times E\big|_+ - \frac{1}{\sqrt{\varepsilon_D}} \nu \times E\big|_- = 0 \quad \text{on } \partial D, \tag{6.1.9c}$$

$$\frac{1}{\sqrt{\mu_0}} \nu \times H\big|_+ - \frac{1}{\sqrt{\mu_D}} \nu \times H\big|_- = 0 \quad \text{on } \partial D, \tag{6.1.9d}$$

$$\begin{pmatrix} E^s \\ H^s \end{pmatrix} = \begin{pmatrix} E - E^i \\ H - H^i \end{pmatrix} \quad \text{satisfies SMRC}, \tag{6.1.9e}$$

where (E^i, H^i) satisfies (6.1.9b) in $\mathbb{R}^3$. We define the scaling matrix $\mathbf{S}$ by

$$\mathbf{S} = \begin{pmatrix} \frac{\sqrt{\varepsilon_0}}{\sqrt{\varepsilon_D}} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \frac{\sqrt{\mu_0}}{\sqrt{\mu_D}} \mathbf{I} \end{pmatrix}.$$

Then the transmission conditions (6.1.9c) and (6.1.9d) read as

$$\begin{pmatrix} \gamma_t^+ (E^s + E^i) \\ \gamma_N^+ (E^s + E^i) \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{\varepsilon_0}}{\sqrt{\varepsilon_D}} \gamma_t^- E \\ \frac{\sqrt{\mu_0}}{\sqrt{\mu_D}} \gamma_N^- E \end{pmatrix} = \mathbf{S} \begin{pmatrix} \gamma_t^- E \\ \gamma_N^- E \end{pmatrix}. \tag{6.1.10}$$

Let $\mathbf{C}^+$ be the exterior Calderón projector with respect to the exterior wavenumber k and $\mathbf{C}^-$ the interior Calderón projector with respect to the interior wavenumber κ, i.e.

$$\mathbf{C}^+ = \frac{1}{2}\mathbf{I} - \mathbf{A}_k, \quad \mathbf{C}^- = \frac{1}{2}\mathbf{I} + \mathbf{A}_\kappa.$$

Then we have by Theorem 6.5

$$\mathbf{C}^+ \begin{pmatrix} \gamma_t^+ E^s \\ \gamma_N^+ E^s \end{pmatrix} = \begin{pmatrix} \gamma_t^+ E^s \\ \gamma_N^+ E^s \end{pmatrix}, \quad \mathbf{C}^- \begin{pmatrix} \gamma_t^- E \\ \gamma_n^- E \end{pmatrix} = \begin{pmatrix} \gamma_t^- E \\ \gamma_N^- E \end{pmatrix}.$$

We apply this to (6.1.10) to get

$$\mathbf{S}\mathbf{C}^- \begin{pmatrix} \gamma_t^- E \\ \gamma_N^- E \end{pmatrix} = \mathbf{C}^+ \begin{pmatrix} \gamma_t^+ E^s \\ \gamma_N^+ E^s \end{pmatrix} + \begin{pmatrix} \gamma_t^+ E^i \\ \gamma_N^+ E^i \end{pmatrix}.$$

We apply again the transmission condition (6.1.10) to remove the interior traces and get

$$\mathbf{S}\mathbf{C}^{-}\mathbf{S}^{-1}\begin{pmatrix}\gamma_t^{+}(E^s+E^i)\\ \gamma_N^{+}(E^s+E^i)\end{pmatrix} = \mathbf{C}^{+}\begin{pmatrix}\gamma_t^{+}E^s\\ \gamma_N^{+}E^s\end{pmatrix} + \begin{pmatrix}\gamma_t^{+}E^i\\ \gamma_N^{+}E^i\end{pmatrix}.$$

We gather the traces of the incoming and the scattered field, to finally have

$$\left(\mathbf{S}\mathbf{A}_\kappa\mathbf{S}^{-1} + \mathbf{A}_k\right)\begin{pmatrix}\gamma_t^{+}E^s\\ \gamma_N^{+}E^s\end{pmatrix} = \left(\frac{1}{2}\mathbf{I} - \mathbf{S}\mathbf{A}_\kappa\mathbf{S}^{-1}\right)\begin{pmatrix}\gamma_t^{+}E^i\\ \gamma_N^{+}E^i\end{pmatrix}, \tag{6.1.11}$$

a boundary integral formulation of (6.1.9a) - (6.1.9e), see also [42]. This integral equation is always uniquely solvable, see [7, Theorem 12] and often called *PMCHWT (Poggio-Miller-Chan-Harrington-Wu-Tsai)*.

Of course, one could remove the exterior traces instead of the interior ones and get a boundary integral formulation, where $\gamma_t^{-}E$ and $\gamma_N^{-}E$ are the unknowns. But from a scattering problem point of view, we are more interested in the scattered field E^s.

6.1.3. Obstacles with impedance boundary condition

Let $D \subset \mathbb{R}^3$ be a bounded Lipschitz domain and let $k > 0$ denote the wavenumber. Recall the scattering problem from an obstacle with impedance boundary condition:

$$\operatorname{curl} E = \mathrm{i}k\,H, \quad \operatorname{curl} H = -\mathrm{i}k\,E \quad \text{in } \mathbb{R}^3 \setminus \overline{D} \tag{6.1.12a}$$

$$\nu \times H = \lambda\big(\nu \times (E \times \nu)\big) \quad \text{on } \partial\Omega \tag{6.1.12b}$$

$$\begin{pmatrix}E^s\\ H^s\end{pmatrix} = \begin{pmatrix}E - E^i\\ H - H^i\end{pmatrix} \quad \text{satisfies SMRC,} \tag{6.1.12c}$$

where (E^i, H^i) is a solution of (6.1.12a) in $\mathbb{R}^3$. We choose the *direct* approach to get an integral equation of (6.1.12a)-(6.1.12c). From the Stratton-Chu formula, see Theorem 6.2, we have

$$E^s(x) = -\mathcal{H}\gamma_t E(x) - \mathcal{E}\gamma_N E(x), \quad x \in \mathbb{R}^3 \setminus \overline{D}. \tag{6.1.13}$$

Since the incoming field (E^i, H^i) is a solution of the Maxwell system (6.1.12a) in D, we have again by the Stratton-Chu formula

$$0 = -\mathcal{H}\gamma_t E^i(x) - \mathcal{E}\gamma_N E^i(x), \quad x \in \mathbb{R}^3 \setminus \overline{D}. \tag{6.1.14}$$

Applying the trace γ_t to (6.1.13) and (6.1.14) and considering the jump relations of the potentials, see Lemma 6.4 yields

$$\gamma_t E = \gamma_t E^i + \gamma_t E^s + 0 = \gamma_t E^i + \big(\frac{1}{2}\mathbf{I} - \mathbf{H}\big)\gamma_t E - \mathbf{E}\gamma_N E.$$

We apply the boundary condition (6.1.12b) to get

$$\frac{1}{2}\gamma_t E + \mathbf{H}\gamma_t E - \mathbf{E}\big[\lambda(\nu \times \gamma_t E)\big] = \gamma_t E^i,$$

or, equivalently formulated for the scattered field

$$\frac{1}{2}\gamma_t E^s + \mathbf{H}\gamma_t E^s - \mathbf{E}\big[\lambda(\nu \times \gamma_t E^s)\big] = \mathbf{E}\big[\gamma_N E^i + \lambda(\nu \times \gamma_t E^i)\big], \qquad (6.1.15)$$

where we have used

$$\Big(\frac{1}{2}\mathbf{I} - \mathbf{H}\Big)\gamma_t E^i - \mathbf{E}\gamma_N E^i = 0,$$

which can be seen from applying the trace γ_t to equation (6.1.14). Note that the only unknown in the integral equation (6.1.15) is the Dirichlet trace $\gamma_t E^s$. The integral equation is called *(impedance boundary condition) electric field integral equation (IBC-EFIE)*, since the unknown is the trace of the electric field, see [38].

This formulation does not require λ to be constant. The main difference to the integral equations of the perfect conductor is the rotation of the trace $\gamma_t E^s$, given by $\nu \times \gamma_t E^s$. Note that the rotation is directly applied to the unknown. An *indirect* approach using some Ansatz would have led to an integral equation, where the rotation is applied to the boundary operator. We chose the integral equation (6.1.15) for our implementation.

6.1.4. Implementational details and examples

In this section, we want to present the results for the implemented integral equations for the scattering from a perfect conductor, from a penetrable obstacle and from an obstacle with impedance boundary condition. The direct and indirect EFIE and MFIE can be implemented in BEMPP by a few lines of code. This, together with preconditioning tools, which allow the use of fast iterative solvers is presented in detail in [46]. An actual implementation in BEMPP of the coupled integral equation (6.1.11) for the scattering from a penetrable obstacle can be found in the tutorials on the homepage of BEMPP (`https://bempp.com`). For the implementation of the integral equation for the scattering from an obstacle with impedance boundary condition (6.1.15), we need additionally the rotation operator R, which is given by

$$R\gamma_T\varphi = \gamma_T\varphi \times \nu = \gamma_t\varphi \qquad (6.1.16)$$

for some vector field φ. Note that

$$R\gamma_t\varphi = \gamma_t\varphi \times \nu = -\gamma_T\varphi.$$

Considering formally

$$\begin{aligned}\int_{\partial D} \gamma_T\varphi \cdot \gamma_t\psi \,\mathrm{d}s &= \int_{\partial D} (\nu \times (\varphi \times \nu)) \cdot (\psi \times \nu) \,\mathrm{d}s \\ &= \int_{\partial D} \varphi \cdot (\psi \times \nu) \,\mathrm{d}s = -\int_{\partial D} \psi \cdot (\varphi \times \nu) \,\mathrm{d}s \\ &= -\int_{\partial D} (\nu \times (\psi \times \nu)) \cdot (\varphi \times \nu) \,\mathrm{d}s = -\int_{\partial D} \gamma_t\varphi \cdot \gamma_T\psi \,\mathrm{d}s,\end{aligned}$$

we see that the negative dual pairing $-\langle \gamma_t\varphi, \gamma_T\psi\rangle_{\partial D}$ between $H^{-\frac{1}{2}}(\mathrm{Div}, \partial D)$ and its dual space $H^{-\frac{1}{2}}(\mathrm{Curl}, \partial D)$, see Theorem 2.5, can be seen as the weak formulation for the rotation operator R and can easily be implemented and tested in BEMPP. For the implementation, see Section B.1 in Appendix B. The convergence plot can be seen in Figure A.1 in Appendix A.

Since we are not only interested in just solving scattering problems, but also want to use the solution to calculate for example the domain derivative, we need to verify the accuracy of our solutions. For an arbitrary scatterer D and incoming wave (E^i, H^i), we do not have an analytic expression for the scattered field and therefore can not verify our solution. Recall the vector wave functions used in Section 2.3.1 to present analytic solutions of the scattering problems. If we chose the scatterer $D = B_R(0)$ and the incoming wave, given by

$$E^i(x) = \alpha_N^M M_N^M(x) + \beta_N^M \frac{1}{\mathrm{i}k} \operatorname{curl} M_N^m(x),$$

for some fixed $N \in \mathbb{N}$ and $|m| \leqslant N$ and coefficients $\alpha_N^M, \beta_N^M \in \mathbb{C}$, then we know the solution, which is just given by

$$E^s(x) = a_N^M N_N^M(x) + b_N^M \frac{1}{\mathrm{i}k} \operatorname{curl} N_N^M(x),$$

where the coefficients a_N^M, b_N^M are given, depending on the scattering problem under consideration, by the Lemmata 2.13 for the perfect conductor, 2.15 for the obstacle with impedance boundary condition, or 2.16 for the scattering from a penetrable obstacle. These functions are well suited for testing the chosen size of the elements of the grid, since they are highly oscillating for large N and M. The resulting convergence plots for the direct MFIE (6.1.8), for the integral equation for the scattering from a penetrable obstacle (6.1.11) and for the integral equation (6.1.15) for the scattering from an obstacle with impedance boundary condition can be seen in the figures A.5, A.6 and A.7. For the implementations of (6.1.8) and (6.1.11), we refer to the tutorials on the homepage of BEMPP (`https://bempp.com`). For the implementation of

(6.1.15) with constant λ, see Section B.2. Note that the accuracy of the solution for incident fields with small N differs significantly from the accuracy of the solution for incident fields with larger N but shows the same behaviour of convergence.

6.2. Numerical evaluation of chiral measures

Recall the far field operator $\mathcal{F}$ from Section 5 for one of the scattering problems stated in Section 2.1, defined by

$$\mathcal{F} : L_t^2(\mathbb{S}^2) \to L_t^2(\mathbb{S}^2),$$
$$\mathcal{F}A(\hat{x}) = \int_{\mathbb{S}^2} E_\infty(\hat{x}, d, A(d))\,\mathrm{d}s(d), \quad \hat{x} \in \mathbb{S}^2,$$

where $E_\infty(\hat{x}, d, A)$ denotes the electric far field pattern E_∞ with respect to an incident plane wave with direction $d \in \mathbb{S}^2$ and amplitude $A \in \mathbb{C}^3$. $\mathcal{F}A$ is the far field pattern with respect to the incident Herglotz wave pair $V[A]$, defined by

$$V[A](x) \int_{\mathbb{S}^2} \begin{pmatrix} A(d) \\ d \times A(d) \end{pmatrix} \mathrm{e}^{\mathrm{i}kd\cdot x}\,\mathrm{d}s(d), \quad x \in \mathbb{R}^3,$$

for $A \in L_t^2(\mathbb{S}^2)$. In order to discretize $\mathcal{F}$, we want to choose a complete orthonormal system in $L_t^2(\mathbb{S}^2)$, which allows an easy calculation of the projected operators $\mathcal{F}^{pq}$, which are given for $p, q \in \{+, -\}$ by

$$\mathcal{F}^{pq} : V^q \to V^p, \quad A \mapsto P^p \mathcal{F} P^q A,$$

where $P^\pm$ is the orthogonal projection from $L_t^2(\mathbb{S}^2)$ onto $V^\pm$ and $V^\pm$ is the eigenspace of the operator $\mathcal{C}A(d) = \mathrm{i}d \times A(d)$ with respect to the eigenvalue ± 1. They satisfy

$$L_t^2(\mathbb{S}^2) = V^+ \oplus V^-, \quad V^+ \perp V^-.$$

Recall the spherical surface harmonics U_n^m, V_n^m, defined for $n \in \mathbb{N}$ and $|m| \leqslant n$ by

$$U_n^m(d) = \frac{1}{\sqrt{n(n+1)}} \operatorname{Grad}_{\mathbb{S}^2} Y_n^m(d), \quad V_n^m(d) = d \times U_n^m(d),$$

which form a complete orthonormal system in $L_t^2(\mathbb{S}^2)$, see Lemma 2.10. We define the linear combinations

$$A_n^m = U_n^m + \mathrm{i}V_n^m, \quad B_n^m = U_n^m - \mathrm{i}V_n^m.$$

Then we have for any $n \in \mathbb{N}$ and $|m| \leqslant n$

$$\mathrm{i}(d \times A_n^m) = \mathrm{i}d \times U_n^m - d \times (d \times U_n^m(d)) = U_n^m(d) + \mathrm{i}V_n^m(d) = A_n^m,$$

i.e. the A_n^m are eigenfunctions of $\mathcal{C}$ with respect to the eigenvalue 1. Analogously, the B_n^m are eigenfunctions of $\mathcal{C}$ with respect to the eigenvalue -1. The sets $\{A_n^m\}$ and $\{B_n^m\}$ form complete orthogonal systems in V^+ and V^-, respectively. They are therefore well suited to discretize $\mathcal{F}$ for our purposes. As a first example, we revisit the scattering from chiral media, see Section 2.1.4.

6.2.1. The chiral ball

Recall the scattering from chiral media in the scaling presented in Section 2.4.3, given by

$$\begin{cases} \operatorname{curl} E = \mathrm{i}k\mu_r(H + \beta_r \operatorname{curl} H) \\ \operatorname{curl} H = -\mathrm{i}k\varepsilon_r(E + \beta_r \operatorname{curl} E) \end{cases} \quad \text{in } \mathbb{R}^3 \setminus \partial D \tag{6.2.1a}$$

$$\nu \times E\big|_+ - \nu \times E\big|_- = 0, \quad \nu \times H\big|_+ - \nu \times H\big|_- = 0 \quad \text{on } \partial D \tag{6.2.1b}$$

$$\begin{pmatrix} E^s \\ H^s \end{pmatrix} = \begin{pmatrix} E - E^i \\ H - H^i \end{pmatrix} \quad \text{satisfies SMRC.} \tag{6.2.1c}$$

Here again, μ_r, ε_r and β_r denote the piecewise constant material parameter, given by

$$\varepsilon_r(x) = \begin{cases} \frac{\varepsilon_D}{\varepsilon_0}, & x \in D \\ 1, & x \notin \overline{D} \end{cases}, \quad \mu_r(x) = \begin{cases} \frac{\mu_D}{\mu_0}, & x \in D \\ 1, & x \notin \overline{D} \end{cases}$$

and

$$\beta_r(x) = \begin{cases} \beta, & x \in D \\ 0, & x \notin \overline{D} \end{cases}.$$

and k denotes the wavenumber. Considering the special case of the chiral ball $D = B_1(0)$, we aim to find an analytic expression of the measure of chirality χ and the smooth measure of chirality χ_{HS}. First, we make some observations. Following [4], we consider the linear combinations

$$E^\pm = E \pm \mathrm{i}H$$

instead of the field (E, H). One finds that $E^\pm$ satisfy the equations

$$\operatorname{curl}\operatorname{curl} E^\pm - k_\pm^2 E^\pm = 0, \quad \text{in } \mathbb{R}^3,$$

where the piecewise constant wavenumber $k_\pm$ is given by

$$k_\pm = \begin{cases} k & \text{in } \mathbb{R}^3 \setminus \overline{D} \\ \kappa^\pm & \text{in } D \end{cases},$$

with
$$\kappa^{\pm} = \frac{\sqrt{\varepsilon_r \mu_r} k}{1 \mp \sqrt{\varepsilon_r \mu_r} k\beta}.$$
This shows, that there are two critical points $\beta_{\text{crit}}^{\pm}$ for the chiral parameter β, namely
$$\beta_{\text{crit}}^{\pm} = \mp \frac{\sqrt{\varepsilon_r \mu_r} - 1}{\sqrt{\varepsilon_r \mu_r} k}.$$
If $\beta = \beta_{\text{crit}}^{\pm}$, then we have $\kappa^{\pm} = k$, i.e. the interior wavenumber for the fields of helicity ± 1 is the same as the exterior wavenumber. In other words, the scatterer is invisible for incident fields of helicity ± 1. We expect the measure of chirality χ and the modified measure of chirality χ_{HS} to be maximal for these values of β. Let $\mathcal{F}$ denote the far field operator with respect to the scattering from chiral media with $D = B_1(0)$. Let the tangential vector field $A \in L_t^2(\mathbb{S}^2)$ be given by
$$A = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} (\alpha_n^m A_n^m + \beta_n^m B_n^m).$$
Then it is shown in [28], that $\mathcal{F}A$ is given by
$$\mathcal{F}A = \frac{(4\pi)^2 \mathrm{i}}{k} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \big(\gamma_n(\kappa^+) \alpha_n^m A_n^m + \gamma_n(\kappa^-) \beta_n^m B_n^m\big),$$
where
$$\begin{aligned} \gamma_n(\kappa) &= \frac{\operatorname{Re} d_n(\kappa)}{d_n(\kappa)} \\ d_n(\kappa) &= \Big(\frac{1}{\kappa} - \frac{1}{k}\Big) j_n(\kappa) h_n^{(1)}(k) + h_n^{(1)}(k) j_n'(\kappa) - j_n(\kappa) h_n^{(1)\prime}(k). \end{aligned}$$
Note that the chiral ball preserves helicity, i.e. we have $\mathcal{F}^{+-} = \mathcal{F}^{-+} = 0$ for any β. $\mathcal{F}$ has the eigenvalues λ_n^1, λ_n^2, $n \in \mathbb{N}$, given by
$$\lambda_n^1 = \mathrm{i}\frac{(4\pi)^2}{k} \gamma_n(\kappa^+), \quad \lambda_n^2 = \mathrm{i}\frac{(4\pi)^2}{k} \gamma_n(\kappa^-), \quad n \in \mathbb{N}.$$
The eigenvalues λ_n^i, $i = 1, 2$ have the multiplicity $2n + 1$. The corresponding eigenfunctions are given by A_n^m for λ_n^1 and by B_n^m for λ_n^2 for $m = -n, \dots, n$. The projected operator $\mathcal{F}^{++}$ and $\mathcal{F}^{--}$ are given by
$$\mathcal{F}^{++} A = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \lambda_n^1 \frac{\langle A, A_n^m \rangle_{L_t^2(\mathbb{S}^2)}}{\|A_n^m\|_{L_t^2(\mathbb{S}^2)}^2} A_n^m$$

$$\mathcal{F}^{--}A = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} \lambda_n^2 \frac{\langle A, B_n^m\rangle_{L_t^2(\mathbb{S}^2)}}{\|B_n^m\|_{L_t^2(\mathbb{S}^2)}^2} B_n^m$$

Note that since $\mathcal{F}$ is diagonal in the orthonormal basis

$$\{A_n^m/\|A_n^m\|_{L_t^2(\mathbb{S}^2)}, B_n^m/\|B_n^m\|_{L_t^2(\mathbb{S}^2)}, \, n \in \mathbb{N}, \, m = -n, \dots, n\},$$

the singular values of $\mathcal{F}$ are given by the absolute value of the eigenvalues. The measure of chirality χ is then given by

$$\begin{aligned}
\chi(\mathcal{F}) &= \Big(\|\mathcal{S}(\mathcal{F}^{++}) - \mathcal{S}(\mathcal{F}^{--})\|_{\ell^2}^2 + \|\mathcal{S}(\mathcal{F}^{+-}) - \mathcal{S}(\mathcal{F}^{-+})\|_{\ell^2}^2\Big)^{\frac{1}{2}} \\
&= \frac{16\pi^2}{k}\Big(\sum_{n=1}^{\infty}\sum_{m=-n}^{n} \big[|\gamma_n(\kappa^+)| - |\gamma_n(\kappa^-)|\big]^2\Big)^{\frac{1}{2}} \\
&= \frac{16\pi^2}{k}\Big(\sum_{n=1}^{\infty}(2n+1)\big[|\gamma_n(\kappa^+)| - |\gamma_n(\kappa^-)|\big]^2\Big)^{\frac{1}{2}}.
\end{aligned}$$

Similarly, the modified measure of chirality χ_{HS} is given by

$$\begin{aligned}
\chi_{\mathrm{HS}}(\mathcal{F}) &= \Big(\|\mathcal{F}\|_{\mathrm{HS}}^2 - 2\big(\|\mathcal{F}^{++}\|_{\mathrm{HS}}\|\mathcal{F}^{--}\|_{\mathrm{HS}} + \|\mathcal{F}^{+-}\|_{\mathrm{HS}}\|\mathcal{F}^{-+}\|_{\mathrm{HS}}\big)\Big)^{\frac{1}{2}} \\
&= \frac{16\pi^2}{k}\Bigg(\sum_{n=1}^{\infty}(2n+1)\big[\gamma_n(\kappa^+)^2 + \gamma_n(\kappa^-)^2\big] \\
&\qquad - 2\Big(\sum_{n=1}^{\infty}(2n+1)\gamma_n(\kappa^+)^2\Big)^{\frac{1}{2}}\Big(\sum_{n=1}^{\infty}(2n+1)\gamma_n(\kappa^-)^2\Big)^{\frac{1}{2}}\Bigg)^{\frac{1}{2}}.
\end{aligned}$$

We can numerically evaluate $\chi(\mathcal{F})$ and $\chi_{\mathrm{HS}}(\mathcal{F})$ by cutting off these series at some $N \in \mathbb{N}$. In Figure A.8, we plotted the graph of the normalized squared measure of chirality and also the normalized squared modified measure of chirality subject to the chiral parameter $\beta \in (0, \beta_{\mathrm{crit}}^-)$. As expected, we have $\chi(\mathcal{F}) = 0$ for $\beta = 0$ and therefore also $\chi_{\mathrm{HS}}(\mathcal{F}) = 0$; and $\chi(\mathcal{F}) = 1$ for $\beta = \beta_{\mathrm{crit}}^-$ and therefore $\chi_{\mathrm{HS}}(\mathcal{F}) = 1$ for $\beta = \beta_{\mathrm{crit}}^-$. This behaviour illustrates Lemmata 5.11 and 5.12. Also, we can see $\chi_{\mathrm{HS}}(\mathcal{F}) \leqslant \chi(\mathcal{F})$. The measure of chirality $\chi(\mathcal{F})$ has a critical point at $\hat{\beta}$, where it seems to be not differentiable. The reason for this is, that for $\beta = \hat{\beta}$, we have $\gamma_n(\kappa^-) \approx 0$ except for a few $n \in \mathbb{N}$. Note that the modified measure of chirality $\chi_{\mathrm{HS}}(\mathcal{F})$ is smooth at $\hat{\beta}$, but significantly lower. Figure A.9 shows the same situation as Figure A.8, but zoomed in in a neighborhood of β_{crit}^-. Note that neither $\chi(\mathcal{F})$ nor $\chi_{\mathrm{HS}}(\mathcal{F})$ are differentiable in β_{crit}^-, which was expected, since $\mathcal{F}^{--}$ vanishes for $\beta = \beta_{\mathrm{crit}}^-$.

6.2.2. Chiral configuration of achiral spheres

For more complex geometries, there are no analytic expressions of $\chi_{\mathrm{HS}}(\mathcal{F})$ and $\chi(\mathcal{F})$ available. We have to rely on discretizations of the far field operator $\mathcal{F}$ and use the singular values of the discretization in order to calculate $\chi(\mathcal{F})$ and $\chi_{\mathrm{HS}}(\mathcal{F})$. In the following, let $\mathcal{F}$ be the far field operator with respect to the scattering from a perfect conductor, a penetrable obstacle or an obstacle with impedance boundary condition. Numerical solutions with respect to these scattering problems were presented in Section 6.1. Since the far field $\mathcal{F}$ maps the space $L^2_t(\mathbb{S}^2)$ onto itself, we get a natural discretization by considering for some fixed $N \in \mathbb{N}$

$$\mathcal{F} : V_N \to V_N,$$

where the $2N^2 + 4N$ dimensional space V_N is given by

$$V_N = \operatorname{span}\{U_n^m, V_n^m : n \leqslant N, |m| \leqslant n\} \subset L^2_t(\mathbb{S}^2).$$

For every tangential vector field U_n^m, V_n^m with $n \leqslant N$ and $|m| \leqslant n$, we have to solve the scattering problem with the incident field given by the Herglotz wave pair $V[U_n^m]$ and $V[V_N^m]$, respectively. Since a Herglotz wave pair $V[A]$ with $A \in L^2_t(\mathbb{S}^2)$ is a superposition of plane waves, i.e.

$$V[A](x) = \int_{\mathbb{S}^2} \begin{pmatrix} A(d) \\ d \times A(d) \end{pmatrix} \mathrm{e}^{\mathrm{i}kd\cdot x} \,\mathrm{d}s(d), \quad x \in \mathbb{R}^3,$$

we consider first the expansion of a plane wave into vector wave functions, i.e. for some $p \in \mathbb{C}^3$ and $d \in \mathbb{S}^2$ with $d \cdot p = 0$, we consider

$$p\,\mathrm{e}^{\mathrm{i}kd\cdot x} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \Big(\alpha_n^m M_n^m(x) + \beta_n^m \frac{1}{\mathrm{i}k} \operatorname{curl} M_n^m(x) \Big). \tag{6.2.2}$$

In order to find expressions for the unknown coefficients α_n^m and β_n^m, recall the definition of the vector wave functions. We have

$$M_n^m(x) = -j_n(k|x|) V_n^m(x/|x|), \quad x \in \mathbb{R}^3$$

and

$$\begin{aligned} \frac{1}{\mathrm{i}k} \operatorname{curl} M_n^m(x) = {} & \frac{\sqrt{n(n+1)}}{\mathrm{i}k|x|} j_n(k|x|) Y_n^m(x/|x|) \frac{x}{|x|} \\ & + \frac{1}{\mathrm{i}k|x|} \big(j_n(k|x|) + k|x| j_n'(k|x|) \big) U_n^m(x/|x|), \quad x \in \mathbb{R}^3. \end{aligned}$$

We define $\widehat{x} = x/|x|$ and multiply the equation (6.2.2) with $\overline{U_n^m}(\widehat{x}) = U_n^{-m}(\widehat{x})$ and $\overline{V_n^m}(\widehat{x}) = V_n^{-m}(\widehat{x})$ and integrate with respect to $\widehat{x}$ over the unit sphere $\mathbb{S}^2$. Since the U_n^m and V_n^m form an orthonormal system, this yields

$$\int_{\mathbb{S}^2} p \cdot V_n^{-m}(\widehat{x}) \mathrm{e}^{\mathrm{i}k|x|d\cdot\widehat{x}} \,\mathrm{d}s(\widehat{x}) = -\alpha_n^m j_n(k|x|), \tag{6.2.3}$$

$$\int_{\mathbb{S}^2} p \cdot U_n^{-m}(\widehat{x}) \mathrm{e}^{\mathrm{i}k|x|d\cdot\widehat{x}} \,\mathrm{d}s(\widehat{x}) = \beta_n^m \Big(\frac{1}{\mathrm{i}k|x|} j_n(k|x|) + \frac{1}{\mathrm{i}} j_n'(k|x|) \Big). \tag{6.2.4}$$

Recall a Herglotz wave pair $V[A]$ for $A \in L_t^2(\mathbb{S}^2)$ being the superposition of electromagnetic plane waves. We call $v[g]$ for $g \in L^2(\mathbb{S}^2)$ given for $x \in \mathbb{R}^3$ by

$$v[g](x) = \int_{\mathbb{S}^2} g(d) \mathrm{e}^{\mathrm{i}kx\cdot d} \,\mathrm{d}s(d)$$

a *(acoustic) Herglotz wave function.* We identify the left hand sides as Herglotz wave functions, evaluated at $|x|d \in \mathbb{R}^3$, i.e.

$$\int_{\mathbb{S}^2} p \cdot V_n^{-m}(\widehat{x}) \mathrm{e}^{\mathrm{i}k|x|d\cdot\widehat{x}} \,\mathrm{d}s(\widehat{x}) = v[p \cdot V_n^{-m}](|x|d),$$

$$\int_{\mathbb{S}^2} p \cdot U_n^{-m}(\widehat{x}) \mathrm{e}^{\mathrm{i}k|x|d\cdot\widehat{x}} \,\mathrm{d}s(\widehat{x}) = v[p \cdot U_n^{-m}](|x|d).$$

In order to determine the coefficients α_n^m, β_n^m, we consider the asymptotic behaviour of the left and right hand side in (6.2.3) and (6.2.4). For the Herglotz wave functions on the left hand side, we have for $x = rd$, with $r > 0$ and $d \in \mathbb{S}^2$ the asymptotic behavior

$$v[g](rd) = -\frac{2\pi\mathrm{i}}{k} g(d) \frac{\mathrm{e}^{\mathrm{i}kr}}{r} + \frac{2\pi\mathrm{i}}{k} g(-d) \frac{\mathrm{e}^{-\mathrm{i}kr}}{r} + \mathcal{O}\Big(\frac{1}{r^2}\Big)$$

for $r \to \infty$, see [3]. For the spherical Bessel function j_n and its derivative j_n', we use the asymptotic behaviour for the spherical Hankel functions of the first and second kind, see (2.3.6), together with the relation

$$j_n(t) = \frac{1}{2} h_n^{(1)}(t) + \frac{1}{2} h_n^{(2)}(t), \quad t \neq 0,$$

to find

$$j_n(kr) = \frac{(-\mathrm{i})^{n+1}}{2k} \frac{\mathrm{e}^{\mathrm{i}kr}}{r} - \frac{\mathrm{i}^{n+1}}{2k} \frac{\mathrm{e}^{-\mathrm{i}kr}}{r} + \mathcal{O}\Big(\frac{1}{r^2}\Big),$$

$$j_n'(kr) = \frac{(-\mathrm{i})^{n}}{2k} \frac{\mathrm{e}^{\mathrm{i}kr}}{r} + \frac{\mathrm{i}^{n}}{2k} \frac{\mathrm{e}^{-\mathrm{i}kr}}{r} + \mathcal{O}\Big(\frac{1}{r^2}\Big)$$

for $r \to \infty$, see [14, Section 2.4]. We compare the coefficients in front of $\frac{\mathrm{e}^{\pm \mathrm{i}kr}}{r}$ in (6.2.3), which yields

$$\begin{aligned} \alpha_n^m &= -4\pi\, \mathrm{i}^n\, p \cdot V_n^{-m}(d), \\ \alpha_n^m &= -4\pi(-\mathrm{i})^n\, p \cdot V_n^{-m}(-d). \end{aligned}$$

Since $V_n^{-m}(-d) = (-1)^n V_n^{-m}(d)$, see [33, Lemma 2.12], we conclude

$$\alpha_n^m = -4\pi\, \mathrm{i}^n \left(p \cdot V_n^{-m}(d)\right), \quad n \in \mathbb{N}, |m| \leqslant n.$$

Similarly, we conclude

$$\beta_n^m = 4\pi\, \mathrm{i}^n \left(p \cdot U_n^{-m}(d)\right), \quad n \in \mathbb{N}, |m| \leqslant n.$$

In conclusion, we have for a plane wave the expansion

$$p\, \mathrm{e}^{\mathrm{i}kd\cdot x} = -4\pi \sum_{n=1}^{\infty} \mathrm{i}^n \sum_{m=-n}^{n} \Big(\big(p \cdot V_n^{-m}(d)\big) M_n^m(x) - \big(p \cdot U_n^{-m}(d)\big) \frac{1}{\mathrm{i}k} \operatorname{curl} M_n^m(x) \Big)$$

into vector wave functions. We insert this representation into the definition of the Herglotz wave pair, which yields for the electric field the expansion

$$\begin{aligned} E[A](x) = -4\pi \sum_{n=1}^{\infty} \mathrm{i}^n \sum_{m=-n}^{n} \Big(&(A, V_n^m)_{L^2(\mathbb{S}^2)} M_n^m(x) \\ &+ (A, U_n^m)_{L^2(\mathbb{S}^2)} \frac{1}{\mathrm{i}k} \operatorname{curl} M_n^m(x) \Big). \end{aligned}$$

Recall that we want to discretize the far field operator by considering the basis

$$\mathcal{B} = \{U_n^m, V_n^m : n \leqslant N, |m| \leqslant n\}$$

for some fixed $N \in \mathbb{N}$. Given an element $A_N \in V_N$, i.e.

$$A = \sum_{n=1}^{N} \sum_{m=-n}^{n} \left(u_n^m U_n^m + v_n^m V_n^m\right),$$

we have found a representation for the corresponding incident field, namely

$$E^i(x) = -4\pi \sum_{n=1}^{N} \mathrm{i}^n \sum_{m=-n^n} \Big(v_n^m M_n^m(x) - u_n^m \frac{1}{\mathrm{i}k} \operatorname{curl} M_n^m(x) \Big),$$

which we use to evaluate the incident field on the boundary of the obstacle. Note, that we can use our numerical experiments from Section 6.1, in order to choose an appropriate $N \in \mathbb{N}$, since they involved exactly these incident fields. By expanding the far field pattern E^∞ as well with respect to elements of $\mathcal{B}$, we arrive at a discretization of the far field operator $\mathcal{F}$ with respect to the basis $\mathcal{B}$. If we order the basis $\mathcal{B}$ by

$$\mathcal{B} = \{U_1^{-1}, U_1^0, U_1^1, U_2^{-2}, \dots, U_N^N, V_1^{-1}, \dots, V_N^N\},$$

we arrive at a representation matrix of the discrete far field operator $\mathcal{F} \in \mathbb{C}^{(2N^2+4N)\times(2N^2+4N)}$, given by

$$\mathcal{F} = \begin{pmatrix} UU & UV \\ VU & VV \end{pmatrix},$$

with UU, UV, VU, $VV \in \mathbb{C}^{(N^2+2N)\times(N^2+2N)}$. The first letter of the block corresponds to the expansion of the far field into U_n^m or V_n^m and the second letter corresponds to the expansion of the incident field into U_n^m or V_n^m. For example, we have

$$UV_{11} = (\mathcal{F}V_1^{-1}, U_1^{-1})_{L^2(\mathbb{S}^2)}.$$

So by solving $2N^2 + 4N$ scattering problems and expanding each of the far fields into $2N^2 + 4N$ vector spherical harmonics, we arrive at a discretization of the far field operator $\mathcal{F}$. In order to evaluate the chiral measure χ and the modified chiral measure χ_{HS}, we need the far field operator $\mathcal{F}$ decomposed into

$$\mathcal{F} = \begin{pmatrix} \mathcal{F}^{++} & \mathcal{F}^{+-} \\ \mathcal{F}^{-+} & \mathcal{F}^{--} \end{pmatrix}$$

which is the representation with respect to the ordered basis $\widehat{\mathcal{B}}$, given by

$$\widehat{\mathcal{B}} = \{U_n^m + \mathrm{i}V_n^m, U_n^m - \mathrm{i}V_n^m : n \leqslant N, |m| \leqslant n\}$$

The corresponding basis change matrix M, which maps elements of $\mathcal{B}$ onto $\widehat{\mathcal{B}}$ and its inverse can easily be identified by

$$M = \begin{pmatrix} \mathbf{I} & \mathbf{I} \\ \mathrm{i}\mathbf{I} & -\mathrm{i}\,\mathbf{I} \end{pmatrix}, \quad M^{-1} = \frac{1}{2}\begin{pmatrix} \mathbf{I} & -\mathrm{i}\mathbf{I} \\ \mathbf{I} & \mathrm{i}\mathbf{I} \end{pmatrix}.$$

We then have

$$\begin{pmatrix} \mathcal{F}^{++} & \mathcal{F}^{+-} \\ \mathcal{F}^{-+} & \mathcal{F}^{--} \end{pmatrix} = M^{-1}\mathcal{F}M$$

and we can easily calculate the singular values of these operators and therefore the measure of chirality χ and also the modified measure of chirality χ_{HS}. As an example, we have chosen four perfectly conducting spheres with different diameters located on the corner points of a tetrahedron. Recall, that we expect χ to be zero by Theorem 5.2, if the constellation of these spheres is geometrically achiral. To illustrate this, we fix three of the radii by setting $r_1 = \frac{1}{2}$, $r_2 = \frac{1}{\sqrt{2}}$ and $r_3 = 1$ while varying r_4 in the interval $[r_1, r_2]$. If r_4 equals r_1 or r_2, the scatterer becomes geometrically achiral. Figure A.10 shows the configuration of the spheres and Figure A.11 shows the plots of the measure of chirality χ and the modified measure of chirality χ_{HS}, relative to its Hilbert Schmidt norm. Calculations were done with wavenumber $k = \sqrt{10}$ and with $N = 5$, i.e. $\mathcal{F} \in \mathbb{C}^{70\times 70}$. Note, that the overall relative chirality of the four perfectly conducting spheres is very low and far from the theoretical maximal value 1. Also note that each combination of three sphere form an geometrically achiral scatterer, i.e. only the scattering due to multiple scattering of the entire ensemble of all four spheres yields the chiral behaviour. As expected, χ has significantly lower values for the cases $r_4 = r_1$ and $r_4 = r_2$. The modified measure of chirality χ_{HS} is even lower and admits an additional local minimum for $r_4 \approx 0.625$.

6.3. Numerical solutions of inverse scattering problems

Recall the iterative Newton scheme from Section 4. In every iteration $i \in \mathbb{N}$, we need to solve (4.0.6), given by

$$\big(\mathbf{F}'[\partial D^i]^*\mathbf{F}'[\partial D^i] + \alpha\mathbf{I}\big)h = \mathbf{F}'[\partial D^i]^*(E_\infty - \mathbf{F}(\partial D^i)),$$

where $\mathbf{F}'[\partial D^i]h$ is the far field pattern of the domain derivative E' with respect to the scatterer D^i and the perturbation h. In Section 6.1, we presented how to solve scattering problems. Since the domain derivative E' is a radiating solution of Maxwell's equations, we can use the same integral equations used to solve the scattering problem in order to calculate the domain derivative E' by changing the right hand side. Recall the inhomogeneous Dirichlet boundary condition of the domain derivative E' of the perfect conductor, see (3.1.7), given by

$$\nu \times E' = \overrightarrow{\mathrm{Curl}}_{\partial D}(h_\nu E_\nu) - \mathrm{i}kh_\nu\,\gamma_T H, \tag{6.3.1}$$

the inhomogeneous impedance boundary condition of the domain derivative E' of the scatterer with impedance boundary condition, see (3.4.4), given by

$$\begin{aligned}\nu \times H' - \lambda\big(\nu \times (E' \times \nu)\big) &= \overrightarrow{\mathrm{Curl}}_{\partial D}(h_\nu H_\nu) + \lambda\,\mathrm{Grad}_{\partial D}(h_\nu E_\nu)\\ &\quad + h_\nu\Big(\frac{\partial\lambda}{\partial\nu} + \mathrm{i}k - 2\lambda(\mathcal{R} - \kappa)\Big)\gamma_T E + \mathrm{i}k\lambda h_\nu\,\gamma_t H,\end{aligned}$$

and the inhomogeneous transmission conditions of the domain derivative E', H' of the scattering from a penetrable obstacle, see (3.2.3) and (3.2.4), given by

$$\frac{1}{\sqrt{\varepsilon_0}}\nu \times E'\big|_+ - \frac{1}{\sqrt{\varepsilon_D}}\nu \times E'\big|_- = \frac{1}{\sqrt{\varepsilon_0}}\big(\overrightarrow{\operatorname{Curl}}_{\partial D}(h_\nu E_\nu\big|_+) - \mathrm{i}kh_\nu\gamma_T^+ H\big) \\ - \frac{1}{\sqrt{\varepsilon_D}}\Big(\overrightarrow{\operatorname{Curl}}_{\partial D}(h_\nu E_\nu\big|_-) - \mathrm{i}\kappa\gamma_T^- H\Big)$$

and

$$\frac{1}{\sqrt{\mu_0}}\nu \times H'\big|_+ - \frac{1}{\sqrt{\mu_D}}\nu \times H'\big|_- = \frac{1}{\sqrt{\mu_0}}\Big(\overrightarrow{\operatorname{Curl}}_{\partial D}(h_\nu H_\nu|_+) + \mathrm{i}kh_\nu\gamma_T^+ E\Big) \\ - \frac{1}{\sqrt{\mu_D}}\Big(\overrightarrow{\operatorname{Curl}}_{\partial D}(h_\nu H_\nu|_-) + \mathrm{i}\kappa h_\nu\gamma_T^- E\Big).$$

In the following, we will present precisely how we implemented and tested the assembly of these right hand sides. Since we do not have analytic expressions at hand to compare our discretizations to, it is crucial to test every step in order to control the resulting error. We start with the perfect conductor.

The first step in order to calculate the right hand side of (6.3.1) is the calculation of the tangential projection of the magnetic field $\gamma_T H$ and the normal component of the electric field $E_\nu = E \cdot \nu$. If we use a direct approach, the unknown λ of our integral equation is given by $\lambda = \gamma_N E = H \times \nu$. Application of the Rotation operator R, see (6.1.16) for the definition, Section B.1 in Appendix B for the implementation and Figure A.1 in Appendix A for the convergence plot, yields access to $(\nu \times (H \times \nu))$. Using an indirect approach and the Ansätze

$$E^s = -\mathcal{E}\lambda \quad \text{and} \quad E^s = \mathcal{H}\lambda$$

leads with the jump relations from Lemma 6.4 the representations

$$\gamma_N E^s = \Big(\frac{1}{2}\mathbf{I} - \mathbf{H}\Big)\lambda \quad \text{and} \quad \gamma_N E^s = -\mathbf{E}\lambda,$$

respectively. By means of R, we get again access to $(\nu \times (H \times \nu))$. For the normal component of the electric field E_ν, we use the relation (2.2.6) with $F = H$ together with $\operatorname{curl} H = -\mathrm{i}kE$, i.e.

$$\operatorname{Div}_{\partial D}(H \times \nu) = -\mathrm{i}kE_\nu.$$

For a smooth enough tangential vector field U and a scalar function v, we have

$$\int_{\partial D} U \cdot \operatorname{Grad}_{\partial D} v \,\mathrm{d}s = -\int_{\partial D} v \operatorname{Div}_{\partial D} U \,\mathrm{d}s,$$

see (2.2.5). The left hand side can be seen as weak formulation for the negative surface divergence $-\operatorname{Div}_{\partial D}$ and the right hand side as weak formulation for the surface gradient $\operatorname{Grad}_{\partial D}$. The surface gradient and the surface divergence can easily be implemented and tested in BEMPP. For the implementations, see Section B.3 in Appendix B and for an error plot see Figure A.2 in Appendix A. Finally, we need to calculate the product of the normal component of the perturbation h and the normal component of the electric field E, i.e. $h_\nu E_\nu$ and the product of the normal component h and the tangential projection of the magnetic field H, i.e. $h_\nu(\nu \times (H \times \nu))$. Note that h is given analytically, but h_ν, E_ν and $(\nu \times (H \times \nu))$ only as discretizations. In order to represent the discrete product $f \cdot_d g$ of two functions f and g in a chosen basis of functions (ϕ_i), we make the Ansatz

$$f \cdot_d g = \sum_i \alpha_i \phi_i,$$

and consider the L^2 projection of the left and right hand side onto the basis functions ϕ_i, i.e. we solve the linear system

$$\int_{\partial D} \phi_j(x) \cdot (f(x)g(x)) \,\mathrm{d}s(x) = \alpha_i \int_{\partial D} \phi_i(x)\phi_j(x) \,\mathrm{d}s(x), \quad j = 1, \ldots.$$

For the case $f = h_\nu$, $g = E_\nu$, we choose a basis of scalar functions and for $f = h_\nu$, $g = (\nu \times (H \times \nu))$, we choose a basis of vector valued functions. The implementation of this scheme can be seen in Section B.4 in Appendix B and the resulting convergence plot in Figure A.3 in Appendix A. With these tools, we are able to calculate the boundary condition for the domain derivative E' by calculating

$$\nu \times E' = R \operatorname{Grad}_{\partial D}(\mathrm{i}kh_\nu \operatorname{Div}(H \times \nu)) + \mathrm{i}kh_\nu R(H \times \nu),$$

where we have a stable discretization for every operator and since we have access to the trace $H \times \nu$. Note, that we need no additional tools to calculate the inhomogeneous transmission conditions for the domain derivative of the scattering from a penetrable obstacle.

For the scattering from an obstacle with impedance boundary condition, we have calculate additionally the curvature operator $\mathcal{R}$ and the mean curvature κ. Recall the definitions

$$\mathcal{R} = J_\nu \quad \text{and} \quad \kappa = \frac{1}{2}\operatorname{div}(\nu) \quad \text{on } \partial D.$$

From $J_\nu \nu = 0$, see Lemma 3.11, we conclude $\frac{\partial \nu}{\partial \nu} = 0$ and since $\mathcal{R} = \mathcal{R}^\top$ we arrive for any vector field F at

$$\mathcal{R}F = \begin{pmatrix} F \cdot \mathrm{Grad}_{\partial D}\, \nu_1 \\ F \cdot \mathrm{Grad}_{\partial D}\, \nu_2 \\ F \cdot \mathrm{Grad}_{\partial D}\, \nu_3 \end{pmatrix}. \tag{6.3.2}$$

For the mean curvature, we use the relation

$$-\Delta_{\partial D} x_i = 2\,\kappa\,\nu_i, \quad i = 1, \dots, 3,$$

see [37], to calculate

$$-\frac{1}{2}\sum_{i=1}^{3} \nu_i\, \Delta_{\partial D} x_i = -\frac{1}{2}\sum_{i=1}^{3} \kappa\, \nu_i^2 = \kappa|\nu|^2 = \kappa. \tag{6.3.3}$$

The left hand side of (6.3.3) can easily implemented in BEMPP with the tools, we already presented, since it is just the combination of (discrete) summation, multiplication and the application of the Laplace-Beltrami operator $\Delta_{\partial D}$. For the implementation of (6.3.2), we need two additional routines, first, the discrete scalar product between two vector fields and then the mapping, which maps the triple (f_1, f_2, f_3) of scalar functions f_i, $i = 1, \dots, 3$ to the vector field, where the i-th component is given by f_i, $i = 1, \dots, 3$, i.e.

$$f_1, f_2, f_3 \mapsto \begin{pmatrix} f_1 \\ f_2 \\ f_3 \end{pmatrix}.$$

We implement the scalar product and the above mapping in the same way as the product of functions by the means of L^2 projections. The implementations can be seen in Listing 10 and 11 in Appendix B, and an error plot in Figure A.4 in Appendix A.

Finally, we have presented all necessary tools in order to fully discretize the equation presented at the beginning of this section. We finish this chapter and also this thesis by presenting numerous actual reconstructions in the following section.

6.3.1. Reconstructions

We have successfully run reconstructions for penetrable obstacles and impenetrable obstacles, either being a perfect conductor or an obstacle with impedance boundary condition. In each case, we considered exact and also noisy data. The results for the penetrable obstacle have already been published in [21].

For each setting, we considered the following shapes, see Figure 6.1:

1. A rounded cuboid, implicitly given by
$$\left(\frac{x_1}{r_1}\right)^n + \left(\frac{x_2}{r_2}\right)^n + \left(\frac{x_3}{r_3}\right)^n = d^n$$
with some exponent $n \in \mathbb{N}$, positive radius $d > 0$ and side lengths $r_1, r_2, r_3 > 0$.

2. A peanut-shaped object, implicitly given by
$$\left(\frac{x_1}{R(2x_3/d)}\right)^2 + \left(\frac{x_2}{R(2x_3/d)}\right)^2 + x_3^2 = \frac{d^2}{4},$$
with $R : [-1, 1] \to \mathbb{R}$, given by $R(z) = \frac{3}{5} - \frac{2}{5}\cos\left(\frac{\pi}{2}z\right)$.

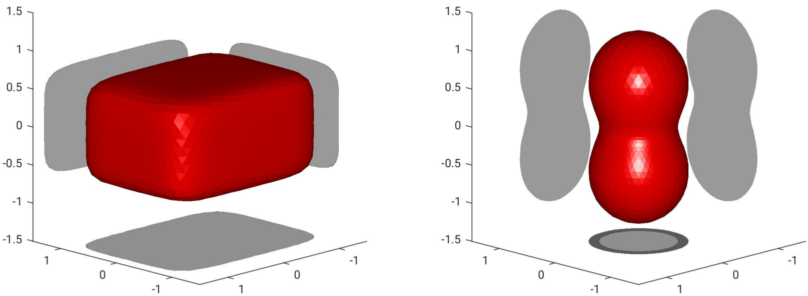

Figure 6.1: The rounded cuboid (on the left) and the peanut shaped object (on the right).

Our implementation requires smooth star shaped objects. Therefore we picked the rounded cuboid to have an object close to the non-smooth cuboid and the peanut-shaped object to test the reconstruction of non-convex objects. In order to cancel possible positive effects due to symmetry, we applied a translation such that the center of the two star shaped objects does not coincide with the center of our star shaped reconstruction in 0. We generated the exact data $E_\infty = \mathbf{F}(\partial D)$ for ∂D being the boundary of the rounded cuboid or the peanut shaped object by picking 168 evaluation points $\hat{x}_i$, $i = 1, \ldots, 168$ on the unit sphere $\mathbb{S}^2$, i.e. the discrete version of E_∞ is an element of $\mathbb{C}^{3\times 168}$. In order to avoid an inverse crime, we ran calculations of the exact data with meshes unrelated to those used in the reconstruction and yielding a higher accuracy. In the case of the perfect conductor, we used also a different integral equation. In the case of noisy data, we multiplied every component of the discrete far field $E_\infty \in \mathbb{C}^{3\times 168}$ with some perturbation factor of the form
$$1 + \delta\lambda_1 \mathrm{e}^{2\pi\mathrm{i}\lambda_2},$$

where λ_1, λ_2 are on $(0,1)$ uniformly distributed random numbers and the *noise level* $\delta \geqslant 0$. We call this *noise up to* δ. The *effective noise level* δ_{eff} is given by

$$\delta_{\text{eff}} = \frac{\|E_\infty - E_\infty^\delta\|}{\|E_\infty\|}.$$

Since the noisy far field E_∞^δ is no longer a (discrete) tangential vector field on the unit sphere $\mathbb{S}^2$, one might think of cancelling the nontangential parts of E_∞^δ before starting the iterative Newton scheme, but since we apply the adjoint of $\mathbf{F}[\partial D^i]$ on the right hand side of (4.0.6), the nontangential parts get canceled automatically. For the calculation of δ_{eff}, we did not see any relevant difference, if we just considered the tangential part of E_∞^δ.

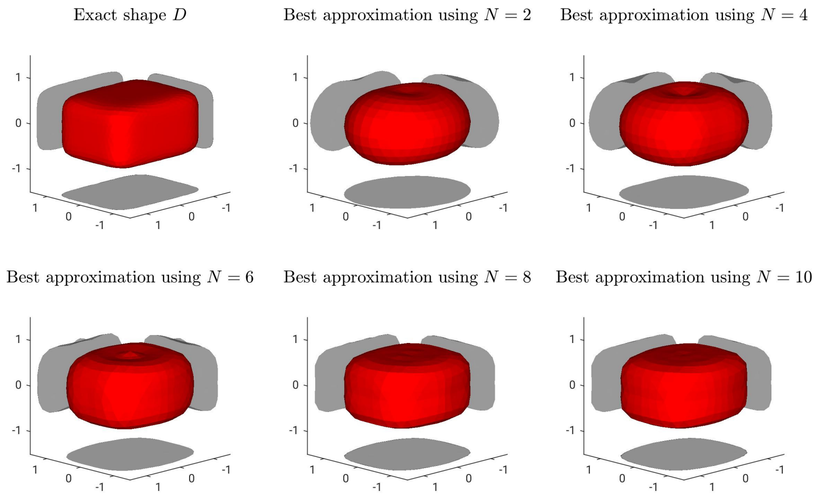

Figure 6.2: Best approximation of the rounded cuboid using $(N+1)^2$ basis functions.

As an initial guess, we have chosen the ball of radius 1, i.e. $D_0 = B_1(0) = \{x \in \mathbb{R}^3, \|x\| \leqslant 1\}$. We have observed that we have to either increase the regularization parameter α drastically or use some a priori information about the size of the scatterer for successful reconstructions. Also, we need the a priori information, that the origin $0 \in \mathbb{R}^3$ is a possible star shaped center.

We have chosen the regularization parameter α by experience. Using too small parameters, especially in the case of noisy data, leads to updates of the parametrization, where negative radii occur, i.e. degenerated objects. But above some critical level, we have observed robust constructions for both scattering objects. Using larger than necessary α slows down the reconstruction speed. In the case of exact data, we have used $\alpha = 3$. In the case of noisy data with $\delta = 0.3$, which lead to $\delta_{\text{eff}} \approx 0.13$, we have used $\alpha = 7$ for the peanut-shaped and $\alpha = 12$ for the rounded cuboid. Reconstructions of the rounded cuboid with $\alpha = 7$ and for the peanut-shaped object with $\alpha = 3$ failed nearly every time.

In order to evaluate the reconstructions, we need to know what is the best reconstruction we can expect. Choosing a fixed number of basis elements for the reconstruction, we can calculate the $L^2(\mathbb{S}^2)$ projection of the parametrization onto these elements. This is, in a sense, the best reconstruction we can hope for. In Figure 6.2, one can see the best approximation of the rounded cuboid using different numbers of basis elements.

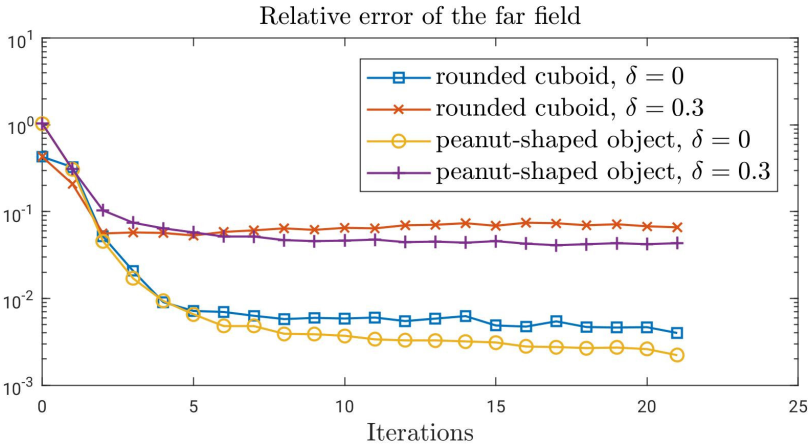

Figure 6.3: Residuals of the reconstruction of the peanut-shaped object and the rounded cuboid with exact and noisy data.

As incident field, we have considered a plane wave (E^i, H^i), given by

$$\begin{pmatrix} E^i \\ H^i \end{pmatrix}(x) = \begin{pmatrix} p \\ d \times p \end{pmatrix} \mathrm{e}^{ikd\cdot x}, \qquad x \in \mathbb{R}^3.$$

To avoid any positive effects due to symmetry of the object with respect to the direction d, we have chosen

$$p = \begin{pmatrix} 1+\mathrm{i} \\ 2 \\ -1+\frac{1}{3}\mathrm{i} \end{pmatrix} \quad \text{and} \quad d = \frac{1}{\sqrt{14}} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

We start by presenting the results for the scattering from a penetrable obstacle. We have chosen the material parameters

$$\varepsilon_r = 2.1, \quad \mu_r = 1.0, \quad k = 1.0472, \quad \kappa = 1.5175,$$

which corresponds to the scattering of Teflon (C_2F_4) illuminated by VHF radiation with wavelength of 6m. We applied noise up to $\delta = 0.3$, which lead to the effective noise level $\delta_{\text{eff}} \approx 0.13$ for the rounded cuboid and $\delta_{\text{eff}} \approx 0.12$ for the peanut-shaped object. We have chosen $N = 7$, i.e. $(N+1)^2 = 64$ basis functions for the reconstructions. In Figure 6.3, the normalized residuals

$$r_i := \frac{\|E_\infty - \mathbf{F}(\partial D^i)\|}{\|E_\infty\|}$$

are plotted. We ran 21 iterations without stopping rule. Observe the relatively large initial error r_0 with $r_0 \approx 1.0$ for the peanut. As expected, after some iterations, the residuals stay on the same level. Note that for exact data, the final errors are significantly lower in comparison to the results for noisy data. In Section A.4 of the Appendix A, the actual reconstructions are presented exemplary after 1, 2, 7 and 21 iterations in Figures A.14 and A.15 for the peanut-shaped object and in Figures A.12 and A.13 for the rounded cuboid. As expected from the residuals, see Figure 6.3, the biggest improvement occurs in the first few iterations. Note, that the algorithm has difficulties in reconstructing the non-convex part of the peanut-shaped object in the case of noisy data. This is due to the high noise level. In Figure A.16 the reconstruction of the peanut-shaped object with $\delta = 0.1$ is presented. Note the much better reconstructed non-convex part but the remaining indention in the direction of the plane wave, which is a known phenomena in inverse acoustic scattering, see [25].

There is hardly any difference in the performance or the result of the reconstructions obtained for penetrable or perfectly conducting obstacles. One might argue, that the reconstruction of the rounded cuboid with impedance boundary condition, as seen in Figure A.17 with $N = 6$, i.e. $(N+1)^2 = 49$ basis functions, with the material parameter

$$k = \frac{\sqrt{5}}{2} \quad \text{and} \quad \lambda = 1.1,$$

with regularization parameter $\alpha = 3$ and the same incident plane wave as before shows a better performance as the reconstructions before, but we do not want to claim that this is the case in general.

A. Figures

A.1. Surface operators

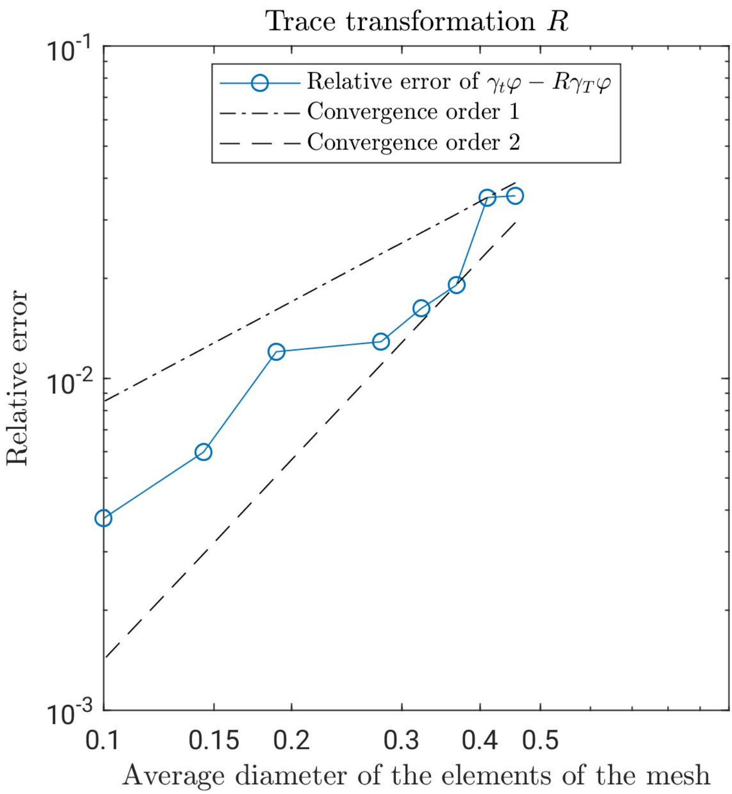

Figure A.1: The relative error between the discretizations of $\gamma_t\varphi$ and $R\gamma_T\varphi$ on the unit sphere with $\varphi(x) = (x_1^2 + x_2, x_2^3, -x_1)^\top$.

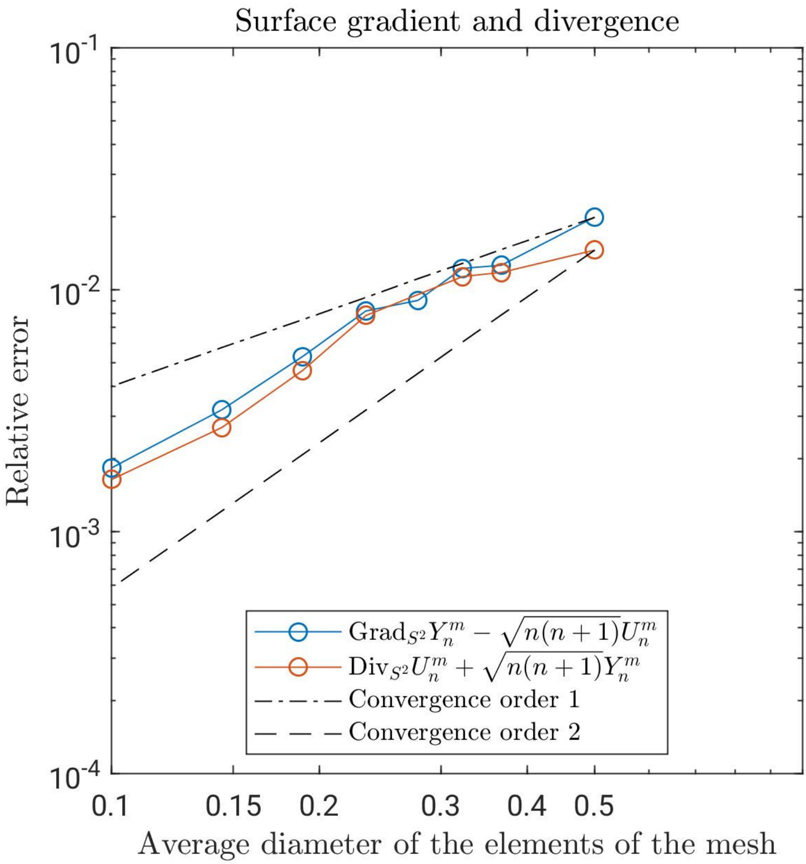

Figure A.2: Relative error of $\mathrm{Grad}_{\mathbb{S}^2} Y_n^m - \sqrt{n(n+1)} U_n^m$ and $\mathrm{Div}_{\mathbb{S}^2} U_n^m + \sqrt{n(n+1)} Y_n^m$ on the unit sphere plotted against the element size h of the mesh for $n = 2$ and $m = 1$.

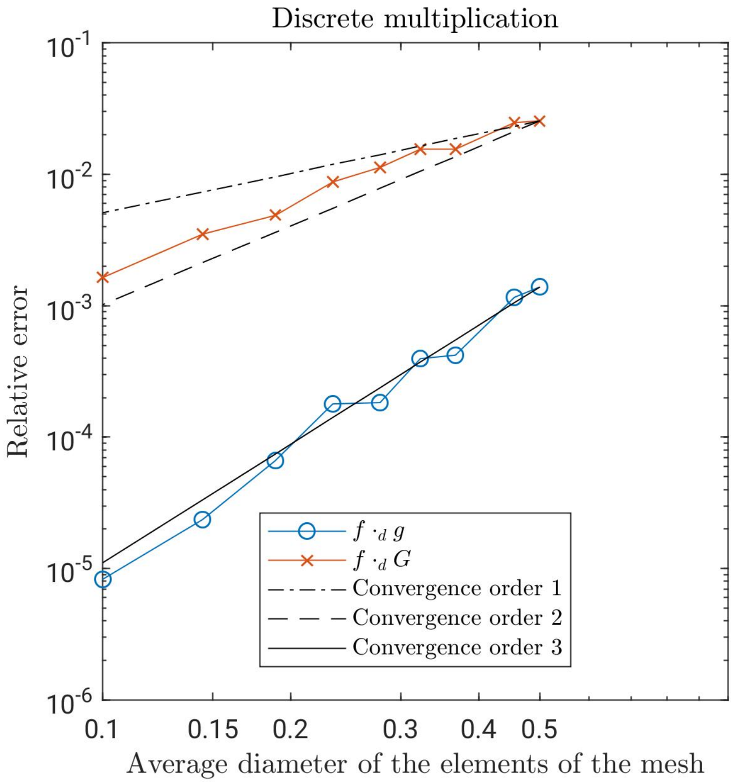

Figure A.3: Relative errors of the discrete multiplication $\cdot_d$ of the functions f and g and of the function f with the vector field G against the element size h of the mesh.

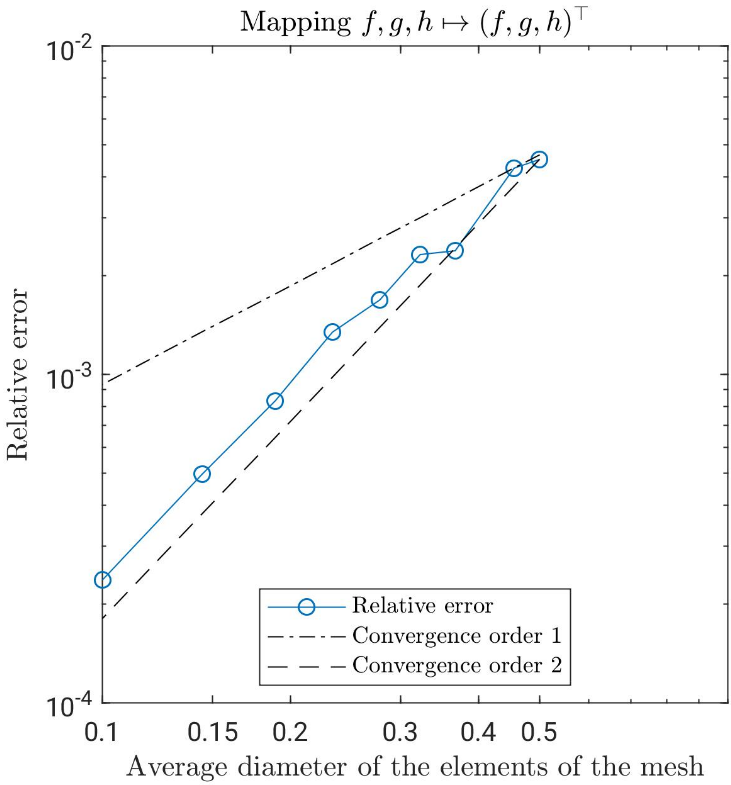

Figure A.4: Relative error of the discrete composition $(f, g, h)^\top$ of the discrete functions f, g, h and the discretized vector field $(f, g, h)^\top$, plotted against the element size h of the mesh.

A.2. Integral equations

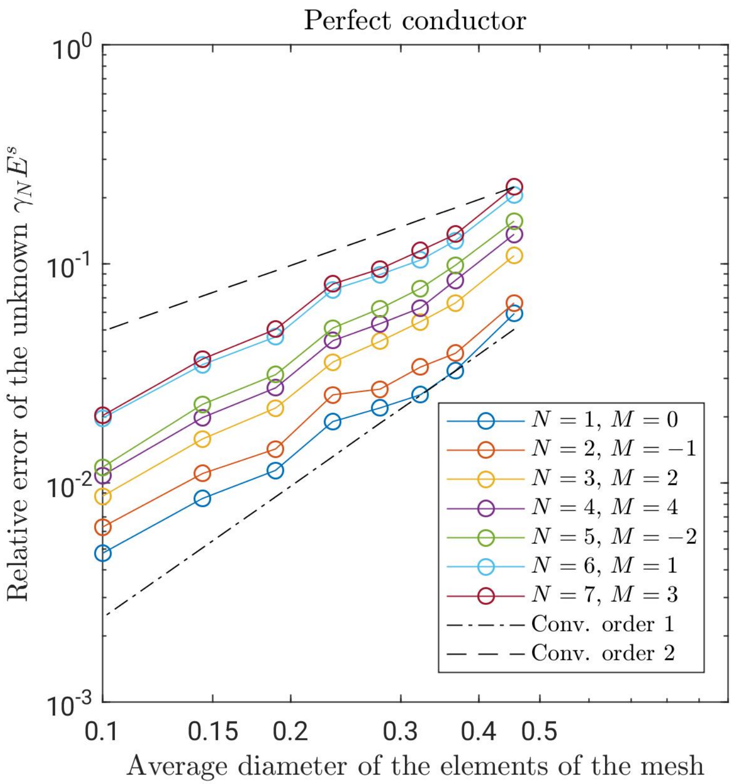

Figure A.5: Scattering from a perfect conducting sphere $\partial D = \partial B_R(0)$ with $R = 1.1$ with wavenumber $k = \sqrt{3.6}$, using the direct MFIE (6.1.8). It is $\alpha_N^M = 2$ and $\beta_N^M = 1.3$.

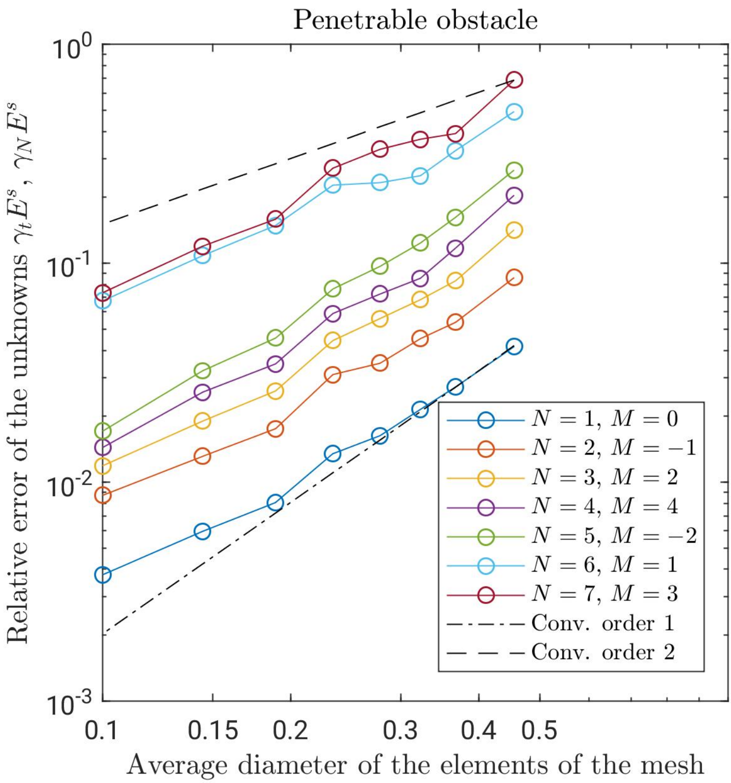

Figure A.6: Scattering from a penetrable sphere $\partial D = \partial B_R(0)$ with $R = 1.1$, with material parameters $\varepsilon_0 = 1.8$, $\varepsilon_D = 1.5$, $\mu_0 = 2.0$, $\mu_D = 1.5$ and $\omega = 1.0$, using the boundary integral equation (6.1.11). It is $\alpha_N^M = 2$ and $\beta_N^M = 1.3$.

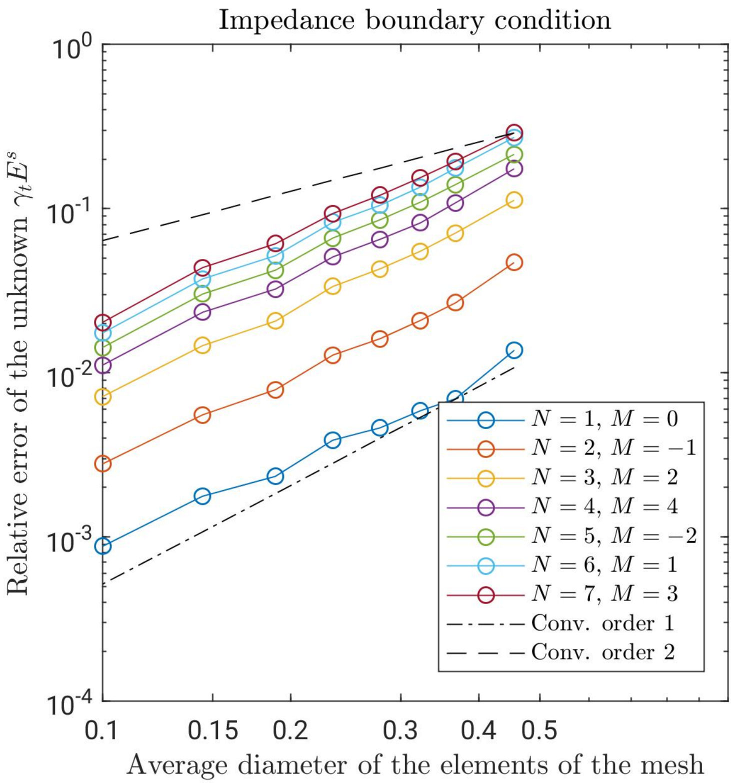

Figure A.7: Scattering from a sphere $\partial D = \partial B_R(0)$ with $R = 1.1$ with impedance boundary condition and constant $\lambda = 0.9$ and wavenumber $k = \sqrt{3.6}$, using the boundary integral equation (6.1.15). It is $\alpha_N^M = 2$ and $\beta_N^M = 1.3$.

A.3. Measuring chirality

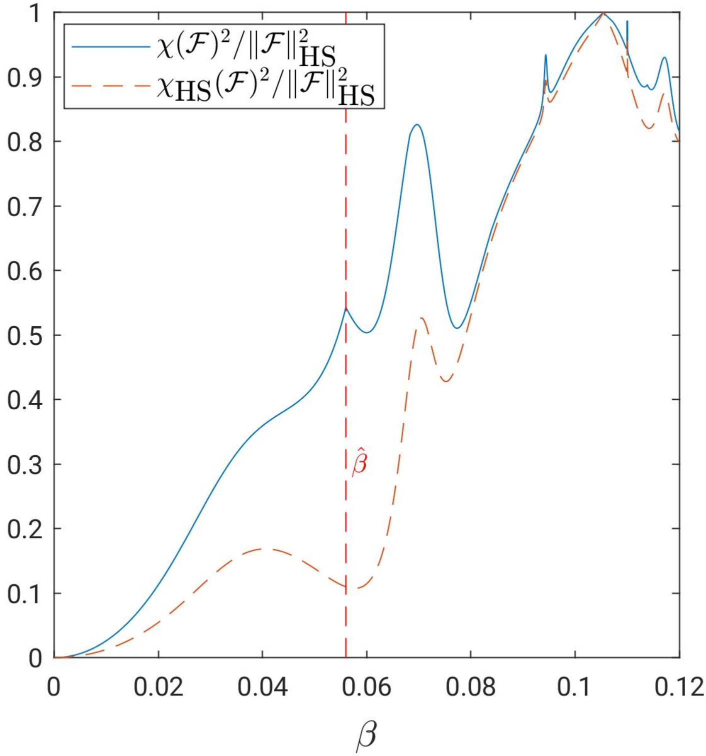

Figure A.8: Relative squared (modified) measure of chirality of the chiral ball $D = B_1(0)$ with $k = \sqrt{10}$ and $\mu_r = \varepsilon_r = 1.5$. The series were cut at $N = 100$.

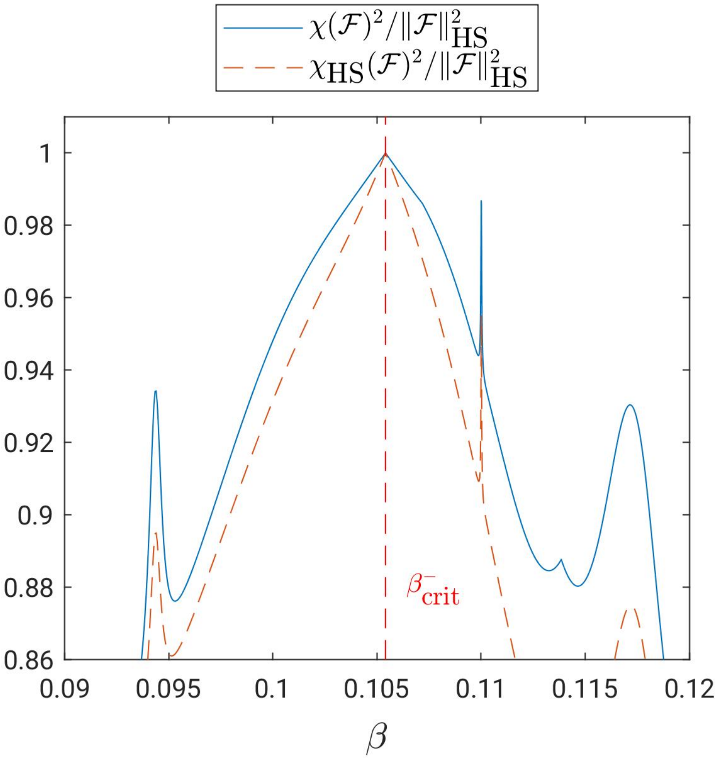

Figure A.9: Relative squared (modified) measure of chirality as in Figure A.8, but zoomed in in the neighborhood of β^-_{crit}.

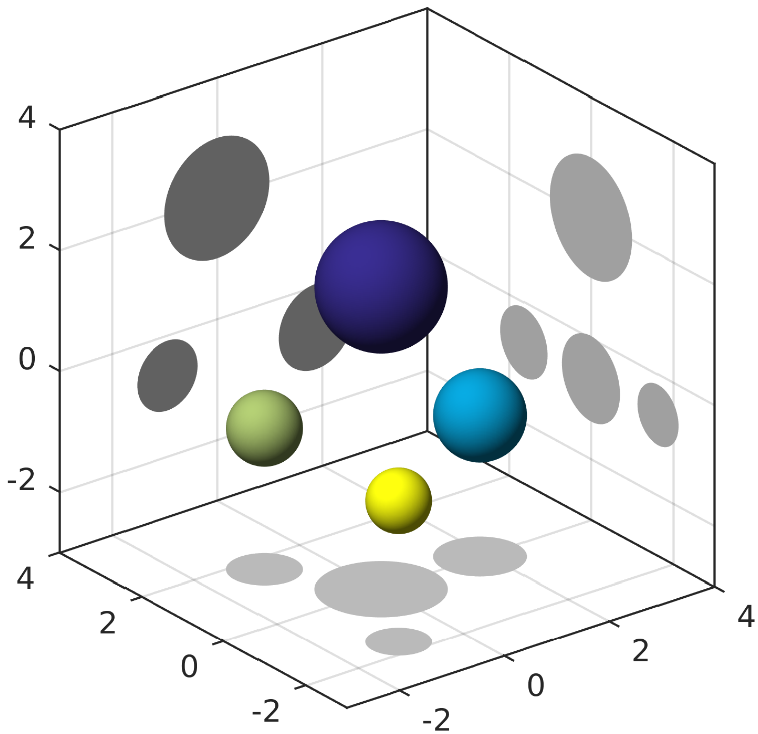

Figure A.10: Geometric constellation of the four perfectly conducting spheres.

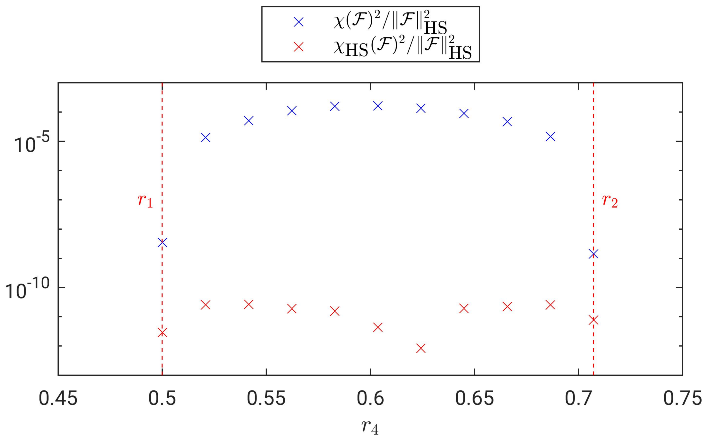

Figure A.11: The relative (modified) measure of chirality in dependency of the radius r_4.

A.4. Reconstructions

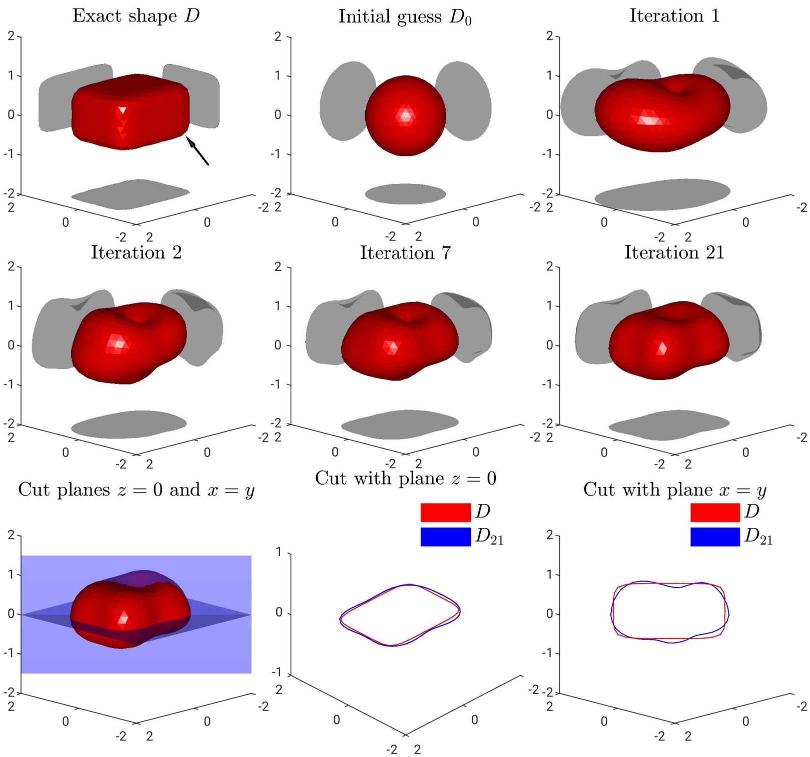

Figure A.12: Reconstructing the rounded cuboid with 64 shape functions and exact data. The black arrow indicates the direction of the incident plane wave.

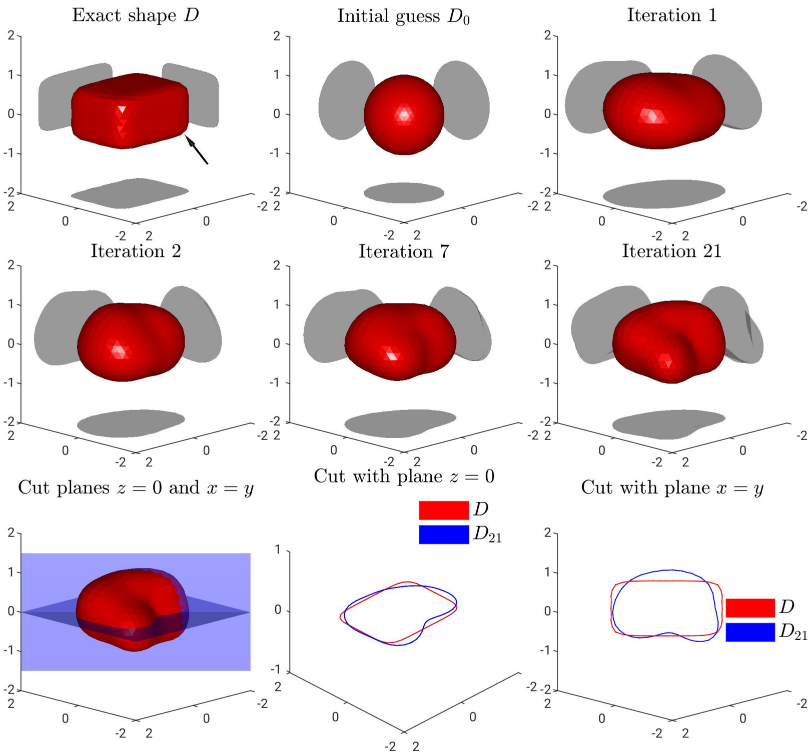

Figure A.13: Reconstructing the rounded cuboid with 64 shape functions and noisy data with $\delta = 0.3$. The black arrow indicates the direction of the incident plane wave.

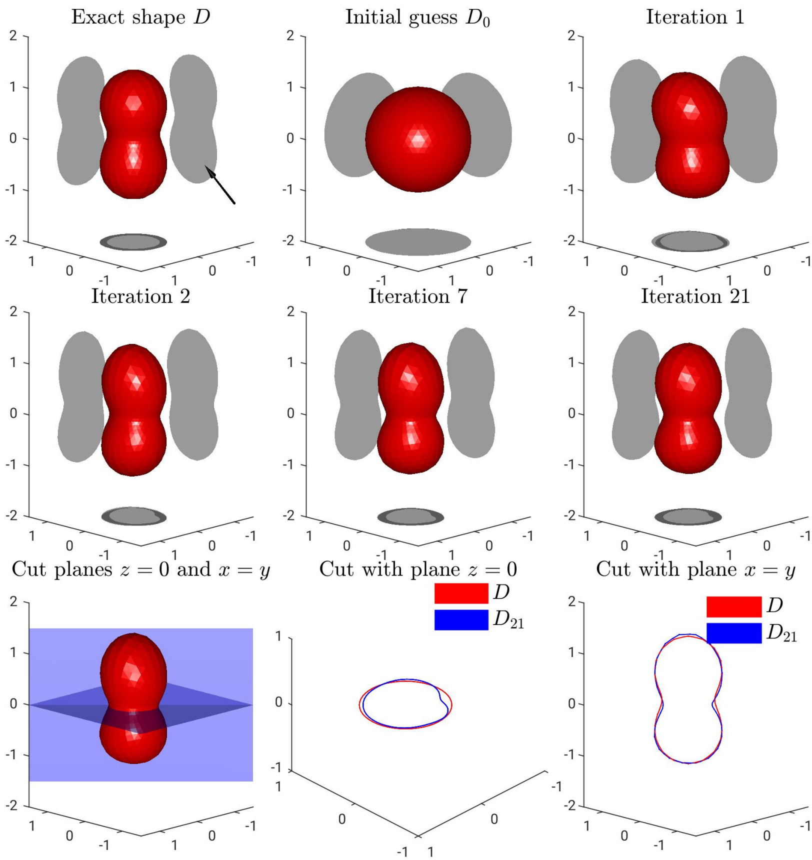

Figure A.14: Reconstruction of the peanut-shaped object with 64 shape functions and exact data.

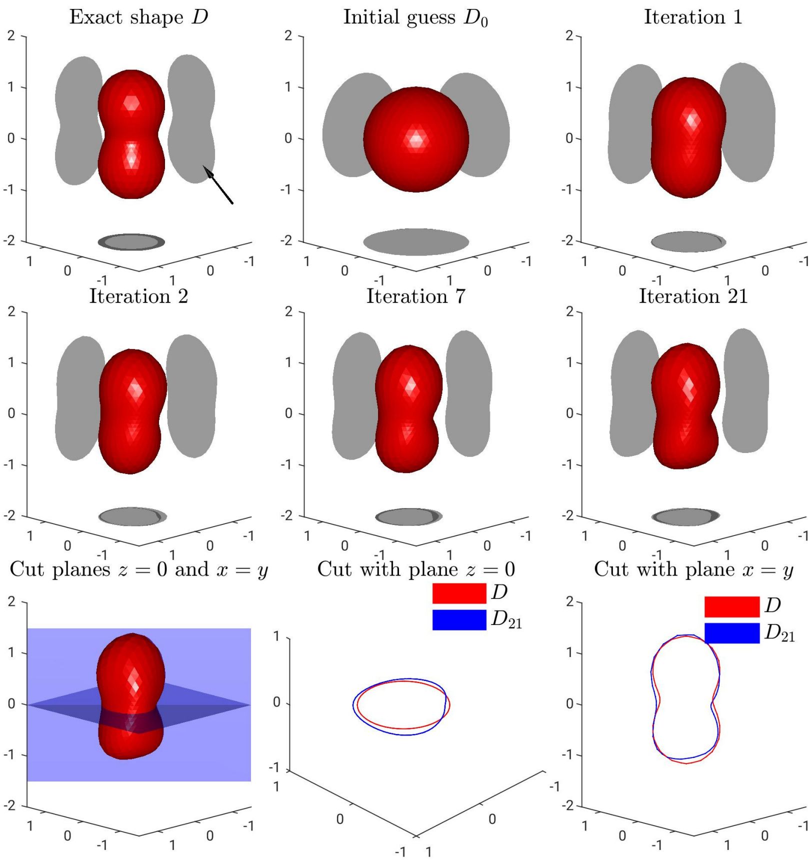

Figure A.15: Reconstruction of the peanut-shaped object with 64 shape functions and noisy data with $\delta = 0.3$.

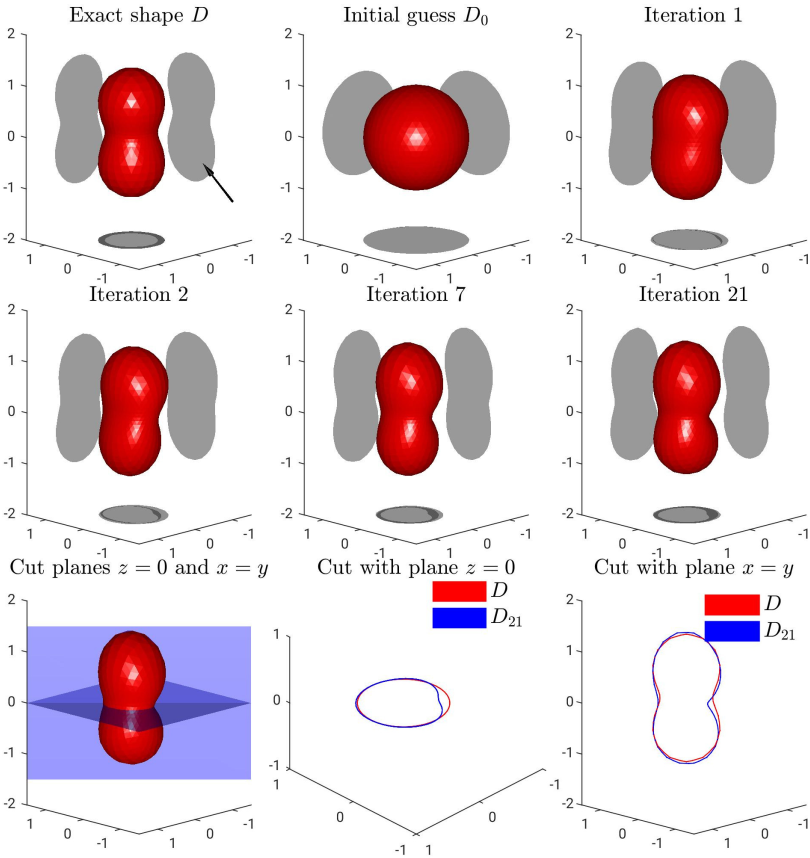

Figure A.16: Reconstruction of the peanut-shaped object with 64 shape functions and noisy data with $\delta = 0.1$.

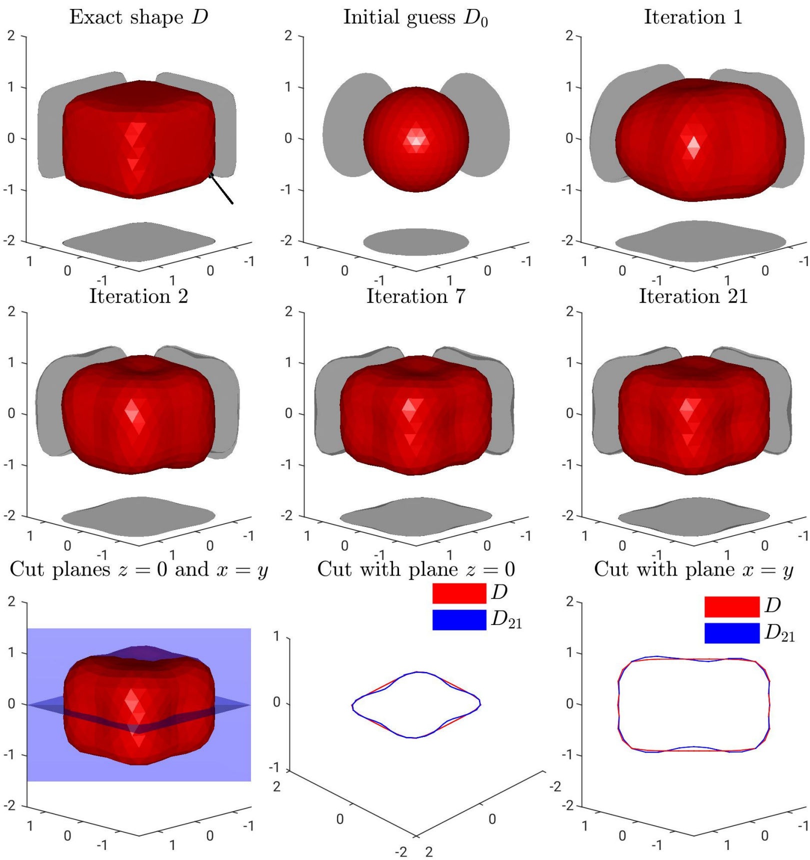

Figure A.17: Reconstruction of the rounded cuboid with impedance boundary condition.

B. Implementations

In this appendix, we want to present some implementations and tools used throughout the thesis to expand the functionality of BEMPP (`https://bempp.com`). Note that these code snippets might not work in future versions. They were implemented and tested with BEMPP 3.3.1 and Python 2.7. We frequently use the Numpy library (`https://numpy.org/`). In order to work, every code snippet needs the following imports:

Listing 1: Basic imports

```python
import bempp.api
import numpy as np
```

B.1. Rotation operator

We start with presenting the implementation of the rotation operator R, defined by

$$R\gamma_T\varphi = \gamma_T\varphi \times \nu = \gamma_t\varphi$$

for some smooth enough vector field φ. This operator can be implemented by the lines presented in the Listing 2.

Listing 2: Implementation of the rotation operator R

```python
def trace_transformation(domain, range_, dual_to_range, label="TRACE_TRANSFORMATION", parameters=None):
    return bempp.api.operators.boundary.sparse._maxwell_identity(domain, range_, dual_to_range, label=label, parameters=parameters)
```

The errors in Figure A.1 were calculated by using Listing 3 and varying the variable `H`, which defines the average diameter of the elements, used for the mesh approximating the unit sphere.

Listing 3: Testing the rotation operator R

```python
H = 0.15
Wavenumber = 1.0
Grid = bempp.api.shapes.sphere(h=H)
MT = bempp.api.operators.boundary.maxwell.multitrace_operator(Grid, Wavenumber)
electric_space, magnetic_space = MT.domain_spaces
electric_dual, magnetic_dual = MT.dual_to_range_spaces
TangentialToTrace = trace_transformation(electric_space, electric_space, electric_dual)
def FunTrace(x,n,d,r):
```

```
    Vector = np.array([x[0]**2 + x[1], x[2]**3, -x[1] ])
    r[:] = np.cross(Vector, n)
def FunTangential(x,n,d,r):
    Vector = np.array([x[0]**2 + x[1], x[2]**3, -x[1] ])
    r[:] = np.cross(n, np.cross(Vector, n))
Tangential = bempp.api.GridFunction(electric_space, fun=FunTangential)
Trace = bempp.api.GridFunction(electric_space, fun=FunTrace)
Test = TangentialToTrace * Tangential
Error = (Test-Trace).l2_norm() / Trace.l2_norm()
```

B.2. IBC-EFIE

Recall the boundary integral equation (6.1.15), given by

$$\frac{1}{2}\gamma_t E^s + \mathbf{H}\gamma_t E^s - \mathbf{E}\big[\lambda(\nu \times \gamma_t E^s)\big] = \mathbf{E}\big[\gamma_N E^i + \lambda(\nu \times \gamma_t E^i)\big].$$

We used the lines presented in Listing 4 to solve this integral equation for constant λ. Note that we have used functions and operators defined above in Appendix B.1, especially the multitrace operator `MT`. The results can be seen in Figure A.7. Lines 6 and 8 have to be filled with the implementations of the Dirichlet trace $\gamma_t E^i$ and Neumann trace $\gamma_N E^i$ respectively.

Listing 4: Implementation of the IBC-EFIE.

```
1  Impedance = 2.0
2  Nu = -trace_transformation(electric_space, magnetic_space, magnetic_dual)
3  ID = bempp.api.operators.boundary.sparse.multitrace_identity(Grid, spaces='maxwell')
4  OP = 0.5 * ID[0,0] + MT[0,0] - Impedance * MT[0,1] * Nu
5  def DirichletIncident(x,n,d,r):
6      r[:] = ... # Define Dirichlet trace .
7  def NeumannIncident(x,n,d,r):
8      r[:] = ... # Define Neumann trace .
9  IncidentTraces = (bempp.api.GridFunction(electric_space, fun=DirichletIncident), bempp.api:GridFunction(magnetic_space, fun=NeumannIncident))
10 rhs_function = IncidentTraces[1] + Impedance * Nu * IncidentTraces[0]
11 RHS = MT[0,1] * rhs_function
12 Solution, _ = bempp.api.linalg.gmres(OP, RHS)
```

B.3. Surface differential operators

Recall the relation (2.2.5), given by

$$\int_{\partial D} v \operatorname{Div}_{\partial D} U \, \mathrm{d}s = -\int_{\partial D} U \cdot \operatorname{Grad}_{\partial D} v \, \mathrm{d}s.$$

We therefore implement the surface gradient by the lines in Listing 5 and analogously the surface divergence in Listing 6.

Listing 5: Implementation of the surface gradient

```
def surface_gradient(domain, range_, dual_to_range,
    label="SURFACE_GRADIENT", symmetry="no_symmetry",
    parameters=None):
    from bempp.api.operators.boundary.sparse import
        operator_from_functors
    from bempp.api.assembly.functors import
        simple_test_trial_integrand_functor
    from bempp.api.assembly.functors import
        surface_divergence_functor
    from bempp.api.assembly.functors import
        scalar_function_value_functor
    return -operator_from_functors(domain, range_, dual_to_range,
        surface_divergence_functor(),
        scalar_function_value_functor(),
        simple_test_trial_integrand_functor(), label, symmetry,
        parameters)
```

Listing 6: Implementation of the surface divergence.

```
def surface_divergence(domain, range_, dual_to_range, label="
   SURFACE_DIVERGENCE", symmetry="no_symmetry", parameters=None):
    from bempp.api.operators.boundary.sparse import
        operator_from_functors
    from bempp.api.assembly.functors import
        hdiv_function_value_functor
    from bempp.api.assembly.functors import
        simple_test_trial_integrand_functor
    from bempp.api.assembly.functors import
        surface_gradient_functor
    return -operator_from_functors(domain, range_, dual_to_range,
        surface_gradient_functor(), hdiv_function_value_functor(),
         simple_test_trial_integrand_functor(), label, symmetry,
        parameters)
```

We use the relations

$$\operatorname{Grad}_{\mathbb{S}^2} Y_n^m = \sqrt{n(n+1)} U_n^m \quad \text{and} \quad \operatorname{Div}_{\mathbb{S}^2} U_n^m = -\sqrt{n(n+1)} Y_n^m$$

in order to test our implementations. The errors in Figure A.2 were calculated by using the lines in Listing 7 and varying the variable `H`, which defines the average diameter of the elements, used for the mesh approximating the unit sphere.

Listing 7: Testing the surface gradient and divergence.

```
H = 0.15
Wavenumber = 1.0
N = 2
M = 1
Grid = bempp.api.shapes.sphere(h=H)
MT = bempp.api.operators.boundary.maxwell.multitrace_operator(Grid, Wavenumber)
VecSpace = MT.domain_spaces[0]
ScaSpace = bempp.api.function_space(Grid, "B-P", 1)
def Ynm(x,n,d,r):
    r[:] = ... # To be filled.
def Unm(x,n,d,r):
    r[:] = ... # To be filled.
fun = bempp.api.GridFunction(ScaSpace, fun=Ynm)
Fun = bempp.api.GridFunction(VecSpace, fun=Unm)
SurfGrad = surface_gradient(ScaSpace, VecSpace, VecSpace)
SurfDiv = surface_divergence(VecSpace, ScaSpace, ScaSpace)
Test1 = SurfGrad * fun
Test2 = SurfDiv * Fun
Error1 = (Test1 - np.sqrt(N*(N+1)) * Fun).l2_norm() / Test1.l2_norm()
Error2 = (Test2 + np.sqrt(N*(N+1)) * fun).l2_norm() / Test2.l2_norm()
```

B.4. Products of functions

The implementation of the product of two functions is given by the code shown in Listing 8. The errors in Figure A.3 were calculated by the lines of code shown in Listing 9 and varying the variable `H`, which again defines the average diameter of the elements, used for the mesh approximating the unit sphere. The functions `fun_1`, `fun_2`, `fun_3` define the three functions f, g, G, given by

$$f(x) = x_1^2 + x_2 - x_1 x_3, \quad g(x) = x_1 x_2 x_3 + x_1 - x_3^2$$

and by

$$G(x) = \nu(x) \times \begin{pmatrix} x_1 x_2 \\ x_2 x_3 \\ x_1 x_3 \end{pmatrix}$$

for $x \in \partial D = \mathbb{S}^2$. We then compute the discrete products fg and fG and compare it to the discretizations of fg and fG, respectively.

Listing 8: Implementation of the discrete multiplication of functions

```
def function_product(f, g, trial_space, test_space):
    from bempp.api.integration import gauss_triangle_points_and_weights
    from bempp.api.utils import combined_type
    accuracy_order = bempp.api.global_parameters.quadrature.far.single_order
    points, weights = gauss_triangle_points_and_weights(accuracy_order)
    if f.space.grid != g.space.grid:
        raise ValueError('f and g must be defined on the same grid')
    element_list = list(test_space.grid.leaf_view.entity_iterator(0))
    dtype = combined_type(f.dtype, g.dtype)
    result = np.zeros(test_space.global_dof_count, dtype=dtype)
    for element in element_list:
        dofs, multipliers =
            test_space.get_global_dofs(element, dof_weights=True)
        n_local_basis_funs = len(multipliers)
        for index in range(n_local_basis_funs):
            coeffs = np.zeros(n_local_basis_funs)
            coeffs[index] = 1
            integration_elements = element.geometry.integration_elements(points)
            basis_values = test_space.evaluate_local_basis(element, points, coeffs)
            f_prod_g = f.evaluate(element, points) * g.evaluate(element, points)
            prod_times_basis = np.sum(f_prod_g * basis_values, axis=0)
            local_res = np.sum(prod_times_basis * weights * integration_elements)
            result[dofs[index]] += multipliers[index] * local_res
    return bempp.api.GridFunction(trial_space,
        dual_space=test_space, projections=result)
```

Listing 9: Testing the discrete multiplication of functions

```
H = 0.15
Grid = bempp.api.shapes.sphere(h=H)
MT = bempp.api.operators.boundary.maxwell.multitrace_operator(Grid, Wavenumber)
VecSpace = MT.domain_spaces[0]
ScaSpace = bempp.api.function_space(Grid, "B-P", 1
def fun_1(x,n,d,r):
    r[0] = x[0]**2 + x[1] - x[2]*x[1]
```

```
def fun_2(x,n,d,r):
    r[0] = x[0] * x[1] * x[2] + x[0] - x[2]**2
def fun_3(x,n,d,r):
    vec = np.array([ x[0] * x[1], x[1] * x[2], x[2] * x[0] ])
    r[:] = np.cross(n, vec)
def fun_p(x,n,d,r):
    r[0] = (x[0]**2 + x[1] - x[2]*x[1]) * (x[0] * x[1] * x[2] + x[0] - x[2]**2)
def fun_P(x,n,d,r):
    vec = np.array([ x[0] * x[1], x[1] * x[2], x[2] * x[0] ])
    r[:] = np.cross(n, vec) * (x[0]**2 + x[1] - x[2]*x[1])
Fun_1 = bempp.api.GridFunction(ScaSpace, fun=fun_1)
Fun_2 = bempp.api.GridFunction(ScaSpace, fun=fun_2)
Fun_3 = bempp.api.GridFunction(VecSpace, fun=fun_3)
Fun_p = bempp.api.GridFunction(ScaSpace, fun=fun_p)
Fun_P = bempp.api.GridFunction(VecSpace, fun=fun_P)
Test_1 = function_product(Fun_1, Fun_2, ScaSpace, ScaSpace)
Test_2 = function_product(Fun_1, Fun_3, VecSpace, VecSpace)
Error_1 = (Test_1-Fun_p).l2_norm() / Test_1.l2_norm()
Error_2 = (Test_2-Fun_P).l2_norm() / Test_2.l2_norm()
```

B.5. Scalar product and composition

The implementation of the scalar product $F \cdot G$ between to vector fields F and G is achieved in the same way as the product of two functions. The only difference lies in choosing a scalar test and trial space and in changing line (20) in Listing 8, such that the local product of F and G is summed up. This is shown in Listing 10.

Listing 10: Implementation of the scalar product.

```
def scalar_product(f, g, trial_space, test_space):
# The same as in function_product.
f_prod_g = np.sum(f.evaluate(element, points) * g.evaluate(element, points), axis=0)
# The same as in function_product.
```

Similarly, we implement the routine, which takes three functions f, g, h and generates vector field $(f, g, h)^\top$ by the lines presented in Listing 11, where we again have to only adapt some lines of Listing 8.

Listing 11: Implementation of the composition.

```
def composition(f, g, h, trial_space, test_space):
# One additional function as argument. The rest as before.
basis_values = test_space.evaluate_local_basis(element, points, coeffs)
fgh = np.zeros((3,3), dtype = dtype)
```

```
fgh[0,0:3] = f.evaluate(element, points)
fgh[1,0:3] = g.evaluate(element, points)
fgh[2,0:3] = h.evaluate(element, points)
prod_times_basis = np.sum(fgh * basis_values, axis=0)
# The rest again as in function_product.
```

In order to test this implementation, we use the lines presented in Listing 12. The errors presented in Figure A.4 were calculated by varying the variable `H`, the size of the elements of the mesh. Note that the discretized function `fgh` and `Test` are tangential vector fields, since the test and trial space consists of tangential vector fields.

Listing 12: Testing the composition mapping.

```
H = 0.15
Wavenumber = 1.0
Grid = bempp.api.shapes.sphere(h=H)
MT = bempp.api.operators.boundary.maxwell.multitrace_operator(Grid
    , Wavenumber)
VecSpace = MT.domain_spaces[0]
ScaSpace = bempp.api.function_space(Grid, "B-P", 1)
def fun_f(x,n,d,r):
    r[0] = 1j * x[0]**2
def fun_g(x,n,d,r):
    r[0] = x[1] - x[2]
def fun_h(x,n,d,r):
    r[0] = x[0]*x[2]*x[1]
def fun_fgh(x,n,d,r):
    r[:] = np.array([ 1j * x[0]**2, x[1] - x[2], x[0]*x[2]*x[1] ])
f = bempp.api.GridFunction(ScaSpace, fun=fun_f)
g = bempp.api.GridFunction(ScaSpace, fun=fun_g)
h = bempp.api.GridFunction(ScaSpace, fun=fun_h)
fgh = bempp.api.GridFunction(VecSpace, fun=fun_fgh)
Test = composition(f, g, h, VecSpace, VecSpace)
Error = (fgh - Test).l2_norm() / fgh.l2_norm()
```

Index

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