Nonlinear Generalized Impedance Boundary Conditions in Inverse Scattering

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Der Mensch empfängt unendlich mehr als er gibt.
Dankbarkeit macht das Leben erst reich.

– Dietrich Bonhoeffer

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Abstract

Nonlinear impedance boundary conditions in acoustic scattering are used as a model for perfectly conductive objects covered with a thin layer of nonlinear medium. In this work, we consider a scattering problem modeled by the Helmholtz equation with a nonlinear generalized impedance boundary condition. For a certain class of nonlinearities, we prove the well-posedness of the nonlinear direct problem and of the associated linearized problem. Furthermore, we show the differentiability of the solution to the scattering problem with respect to the boundary of the scatterer and prove the existence of a domain derivative that satisfies the Helmholtz equation together with a linear impedance boundary condition. A characterization of the domain derivative enables iterative regularization schemes to solve the inverse obstacle scattering problem, which consists of reconstructing the obstacle from the far-field pattern of a scattered wave. Since each iteration step requires solving a nonlinear boundary value problem, we suggest an all-at-once method based on linearizing the scattering problem and applying a regularized Newton step for the reconstruction. We introduce an integral equation method for solving linearized scattering problems and use the Nyström method to compute approximate solutions of the boundary integral equations. Finally, we supplement our theoretical results and the description of the reconstruction algorithm with several examples to illustrate the performance of the proposed scheme.

Contents

Chapter 1

Introduction

1.1. Nonlinear Phenomena in Scattering Theory

Scattering theory generally deals with the effects that obstacles and inhomogeneities have on wave propagation. In this work, we restrict ourselves to time-harmonic waves modeled by the Helmholtz equation in the exterior of the scattering object. Thus, the model may cover acoustic scattering in $\mathbb{R}^3$ as well as a specific polarization in electromagnetic scattering in $\mathbb{R}^2$. An obstacle illuminated by an incident time-harmonic wave responds to the excitation with a scattered wave. Measurement data of the total field, which is a superposition of the incident and scattered waves, can then be collected in the neighborhood of the obstacle. With a priori knowledge of the physical properties of the scatterer and the incident wave, the *direct scattering problem* consists of determining the scattered wave and its behavior at a large distance from the object. Conversely, the question arises of what properties the scatterer must have in order to produce such far-field behavior. If the interest is in reconstructing the shape of the scatterer with knowledge of the far-field pattern, the problem is referred to as the *inverse obstacle scattering problem*. Typically, inverse scattering problems are nonlinear and ill-posed, since the solutions of the problems depend nonlinearly on the given data, and the shape of the scatterer does not depend continuously on the far-field observations of the scattered wave.

In this work, we focus on the reconstruction of an obstacle where the material properties near the boundary can be approximated by an impedance boundary condition with an additional nonlinear term. The modeling of very rough surfaces of highly absorbent media started with the impedance boundary condition introduced by Leontovich in 1948, where the impedance operator is confined to the multiplication with a scalar function. However, impedance conditions containing a second-order (or higher-order) differential operator, also known as generalized impedance conditions, enable the description of physically more complex phenomena and cover a larger number of configurations. Thin layers, whether periodic or not, can be approximated by a generalized impedance condition, which occurs either as a transmission condition (see [ALG99, CHH10]) when the layer lies between two dielectric materials, or as a boundary condition (see [BL96, AH98, HJ02, DHJ06]) when the layer covers a perfectly conductive material. Here, an asymptotic analysis in the thin layer leads to such approximate or effective boundary conditions.

With regard to the inverse scattering problem, the number of unknowns is reduced, because we move from a complex model (thin layer, highly absorbent medium, rough surface, etc.) to a surface model. By using a generalized impedance boundary condition instead of a two-scale model, the inverse problem becomes less ill-posed, see [Cha12]. Throughout this work, we consider a nonlinear surface operator $\mathscr{Z} = \mathscr{Z}_{\text{lin}} + \mathscr{Z}_{\text{nonlin}}$ at the boundary of the scattering object, whose linear part has the form

$$\mathscr{Z}_{\text{lin}} u = \lambda u + \operatorname{Div}(\mu \nabla_\tau u)\,,$$

as proposed in numerous works (see, e.g., [BCH11, BCH12, YZZ14, Kre18, Kre19, Yam19]), where Div denotes the surface divergence, ∇_τ the surface gradient and λ and μ are impedance functions.

Inverse problems have been studied extensively for linear scattering models (see [CK13]), but much less is known about nonlinear media. However, over the last decade, nonlinear phenomena have become increasingly important in acoustic and electromagnetic obstacle scattering, for example, in the case of thinly coated, perfectly conducting objects filled with a nonlinear medium [SSS04, SY10]. Through an asymptotic analysis, nonlinear material properties in thin layers lead to approximate nonlinear boundary conditions [NH99]. Scattering problems with such nonlinear boundary conditions have been studied in [Nic24] for electromagnetic waves and in [BR18, BL19] for the acoustic wave equation, based on boundary element methods in space and convolution quadrature in time. First approaches in recovering the support of nonlinear media can be found in [Lec11, GKM22], where the factorization method and the monotonicity method are employed. These require, at least theoretically, measurements of the far-field pattern for infinitely many incident fields. Throughout this work, however, we assume that we have access to the far-field pattern for a single or just a few incident fields.

Since we are not aware of any previous studies in the field of inverse obstacle scattering problems where the object is characterized by a nonlinear generalized impedance boundary condition, we aim to fill this gap. For the scattering problem with linear impedance boundary conditions, it is observed that iterative regularization schemes based on the domain derivative of the scattering problem lead to feasible reconstruction algorithms (see [BCH12, KR18] and references cited therein). Therefore, in extending this approach to nonlinear generalized impedance boundary conditions, our task is twofold. First, we establish a shape derivative of the scattered field with respect to the scattering obstacle, and second, we develop an iterative regularization scheme for solving the severely ill-posed reconstruction problem.

In view of the variational method for showing the existence of the domain derivative, we introduce a weak scattering theory for the nonlinear boundary condition. To this end, we establish some fairly general assumptions regarding the nonlinear term that ensure a well-posed direct problem. In 1970, Kačurovskii extended the linear Fredholm theory to nonlinear compact operators. We take advantage of this existence result and show that it is applicable to the scattering problem. Furthermore, we rely on Rellich's lemma to obtain a uniqueness and stability statement for the nonlinear scattering problem.

Starting from a well-posed direct problem, we address the question of how solutions to the scattering problem behave with respect to variations of the boundary of the scatterer. Under certain assumptions on the regularity of the boundary and the perturbations, we show that the solutions of the scattering problem are differentiable with respect to the boundary and prove the existence of the material derivative. The approach presented in this work is closely related to the ideas established in [Het22] for semilinear boundary value problems. Similarly to the case of linear boundary value problems, such a derivative can be represented by its domain derivative (see [Kir93, Het95, Het98a, HL18]), which has been shown to satisfy a corresponding linearized impedance boundary value problem for the Helmholtz equation.

With the domain derivative at hand, it is natural to consider iterative regularization schemes for solving the inverse problem. More precisely, the solution of the direct scattering problem with a fixed incident wave defines an operator $\mathcal{F}$ that maps the boundary ∂D of the scatterer onto the far-field pattern u_∞ of the scattered wave. Given a far-field pattern u_∞, the inverse scattering problem consists of solving the nonlinear and ill-posed equation $\mathcal{F}(\partial D) = u_\infty$ for the unknown boundary ∂D. In order to obtain an approximate solution for this nonlinear and ill-posed operator equation, we suggest the use of a regularized Newton-type method.

Inverse scattering problems with linear generalized impedance boundary conditions first emerged in the last 15 years. A reconstruction method for determining the impedance functions λ and μ, based on a method of steepest descent with H^1-regularization of the gradient was presented in [BCH11], where particular emphasis was placed on the case of non regular coefficients and imprecise knowledge of the boundary ∂D. This work was then extended in [BCH12] to the more general inverse problem, where both the shape and the impedance are determined from far-field measurements at a fixed frequency. To determine the shape of an inclusion in a conducting medium, an inverse boundary value problem for the Laplace equation with a generalized impedance boundary condition was considered in [CK12] and further developed in [CHK14]. In this context, a solution method based on boundary integral equations was used, which took both the determination of the unknown boundary and the determination of the unknown impedance functions into account. A similar problem was investigated in [CDK13], where tools for shape optimization by minimizing a least-squares cost functional were utilized for the reconstruction of the inclusion. The factorization method introduced by Kirsch ([Kir89]) was extended in [YZZ14] to the case of generalized impedance boundary conditions to reconstruct a complex obstacle from far-field data at a fixed frequency. Thin dielectric coatings with a variable thickness were first addressed in [AHŞ11], where the reconstruction of the thickness variation of a dielectric coating through generalized impedance boundary conditions was performed by Aslanyürek and Sahintürk in the subsequent work [AŞ14]. An extension of [CK12] by Cakoni and Kress to the Helmholtz equation instead of the Laplace equation was discussed in [Kre18]. Here, an inverse algorithm based on a system of nonlinear boundary integral equations coupled with a single-layer potential approach for solving the forward scattering problem was proposed. The cited works considered the inverse problem only in two dimensions. A first success in three-dimensional reconstruction of the impedance functions was achieved in [Yam19], where the proposed reconstruction algorithm was based on an iterative regularized Newton method and nonlinear integral equations.

Throughout this work, we consider a scattering problem in which nonlinearity arises not only in the inverse problem, but also in the boundary condition of the direct problem. Since any iteration step requires solving a nonlinear boundary value problem, we suggest an all-at-once method based on linearizing the scattering problem and applying a regularized Newton step for the reconstruction. In general, it was shown by Kaltenbacher [Kal16] that such an approach leads to regularization schemes by assuming certain mapping properties of the nonlinear operator. We introduce an integral equation method solving for the linearized scattering problems and develop a Newton-type regularization scheme for the reconstruction of a scattering object from a far-field pattern.

A complete proof of convergence is unfortunately not known even for the inverse object reconstruction for linear scattering problems. For theoretical investigations concerning the stability and convergence of the direct solver in the case of nonlinear boundary conditions, we refer to [WR88, Ruo93, Han95, WC15]. Although the standard assumptions required for convergence theory are not satisfied in the case of inverse scattering problems, we develop an all-at-once approach and show that the proposed method leads to reconstructions that are comparable to the well-known results for linear impedance boundary conditions.

1.2. Outline of the Thesis

The thesis can be divided into two main parts. The first part deals with the direct scattering problem and lays the foundation for the second part, in which an all-at-once Newton-type method for shape reconstruction is elaborated upon.

Part I: Acoustic scattering with nonlinear generalized impedance conditions.

This part provides an introduction to the inverse problem in the context of a nonlinear generalized impedance condition, since we only deal with the direct scattering problem. Chapter 2 begins with preliminaries on the notation of function spaces and necessary elementary definitions. We then proceed with a brief derivation of the model under consideration, consisting of the Helmholtz equation, the Sommerfeld radiation condition, and a nonlinear generalized impedance boundary condition. In Section 2.2.1, we discuss the impedance boundary condition used in more detail by deriving a second-order boundary condition for a specific example from an asymptotic expansion. Our main objective in Sections 2.3 – 2.5 is to prove the well-posedness of the direct problem under various assumptions concerning the impedance functions, the regularity of the boundary, and the nonlinearity. Here we consider that the linearized scattering problem is no longer $\mathbb{C}$-linear, but instead $\mathbb{R}$-linear and thus study the effects of this property in Section 2.4. Subsequently, in Chapter 3, we show the differentiability of solutions to the scattering problem with respect to variations of the boundary. Section 3.1 provides the preparation for the definition of the domain derivative, which is specified in Section 3.2.

Part II: Shape reconstruction.

The consideration of the inverse problem begins in Chapter 4, which aims to reconstruct the shape of the scattered object from information about the far-field pattern (i.e., the field diffracted far away from an obstacle) generated by an incident wave. For this purpose, we introduce a regularized all-at-once Newton-type method in Section 4.2, which performs an update in the linearized forward problem as well as in the linearized and regularized operator equation for the inverse problem at each step. The equations in the discrete form are discussed in more detail in Section 4.3 for the direct problem and in Section 4.4 for the inverse problem. When calculating the synthetic data obtained by solving the forward scattering problem, it is crucial to avoid trivial inversions. Therefore, in Section 4.5, we describe how to compute the synthetic data in order to prevent an *inverse crime*. Furthermore, in Section 4.7, we classify the Newton method used in this work within the context of existing research. Finally, in Chapter 5, we test the performance of the shape reconstruction method on various examples in the unperturbed case as well as with noisy data.

This thesis is supplemented by three appendices: In Appendix A, we derive the calculation steps required for the asymptotic expansion to obtain a nonlinear generalized impedance boundary condition. Appendix B contains the entries of the real matrix representation of the operator to compute the synthetic data and Appendix C provides a representation of the Fréchet derivative of the far-field operator and its adjoint in L^2 in the case of a linear boundary condition.

1.3. Prior Publication

Some results of this work are based on the publication [FH24]. In that paper, the classical impedance boundary conditions in the nonlinear case were considered, while in this thesis, we have extended the findings to nonlinear generalized impedance boundary conditions.

CHAPTER 2

The Direct Problem

2.1. Preliminaries

Initially, we introduce the required function spaces and present important results from the field of functional analysis, to which we will refer repeatedly throughout this thesis. Note that the notation used is predominantly taken from [McL00, KH15].

Let $\Omega \subseteq \mathbb{R}^d$ be an open domain of dimension $d \in \{2, 3\}$, meaning an open connected set that is not necessarily bounded. For the unit sphere in $\mathbb{R}^d$, we use the conventional notation $S^{d-1} := \{x \in \mathbb{R}^d \mid |x| = 1\}$.

A multi-index is a d-tuple $j = (j_1, j_2, \ldots, j_d)$ of non-negative integers, and the order of the multi-index is indicated by the sum $|j| = j_1 + \ldots + j_d$. Given a multi-index j, we define the differential operator by

$$\partial^j := \frac{\partial^{|j|}}{\partial^{j_1} x_1 \ldots \partial^{j_n} x_n} . \tag{2.1}$$

Then, the function spaces that consist of all complex-valued functions whose partial derivatives exist up to the k-th order, for $k \in \mathbb{N}_0 \cup \{\infty\}$ and are continuous on Ω, are denoted by

$$\begin{aligned} C^k(\Omega) &:= \{u \colon \Omega \to \mathbb{C} \mid \partial^j u \text{ is continuous for } |j| \leq k\} , \\ C^k_c(\Omega) &:= \{u \in C^k(\Omega) \mid \operatorname{supp} u \subset \Omega \text{ is compact}\} , \end{aligned}$$

where the support of a function $u \colon \Omega \to \mathbb{C}$ is defined as $\operatorname{supp} u := \overline{\{x \in \Omega \mid u(x) \neq 0\}}$.

By $C^{0,\alpha}(\Omega)$ we denote the space of all bounded and uniformly Hölder-continuous functions on Ω, where a function $u \colon \Omega \to \mathbb{C}$ is uniformly Hölder-continuous with exponent $\alpha \in (0, 1]$ if there exists a constant $C > 0$ such that

$$|u(x) - u(y)| \leq C|x - y|^\alpha \quad \text{for all} \quad x, y \in \Omega.$$

Furthermore, the Hölder space

$$C^{k,\alpha}(\Omega) := \{u \in C^k(\Omega) \mid \exists c > 0 \text{ with } |\partial^j u(x) - \partial^j u(y)| \leq c|x - y|^\alpha \text{ for all } x, y \in \Omega, \ |j| = k\}$$

is defined as the set of functions that are differentiable up to order k, where the k-th derivatives are Hölder-continuous with exponent $\alpha \in (0,1]$. If $\alpha = 1$, the functions are called Lipschitz-continuous.

For $1 \leq p \leq \infty$, the standard Lebesgue space $L^p(\Omega)$ is given by the vector space of equivalence classes of Lebesgue-measurable functions $u\colon \Omega \to \mathbb{C}$ that are p-integrable with respect to the Lebesgue measure. Consequently,

$$L^p(\Omega) := \{u\colon \Omega \to \mathbb{C} \mid u \text{ is Lebesgue measurable and } \|u\|_{L^p(\Omega)} < \infty\}$$

and the corresponding norm is defined by

$$\|u\|_{L^p(\Omega)} := \begin{cases} \left(\int_\Omega |u(x)|^p \,\mathrm{d}x\right)^{\frac{1}{p}}, & \text{for } 1 \leq p < \infty, \\ \operatorname{ess\,sup}_{x\in\Omega} |u(x)|, & \text{for } p = \infty. \end{cases}$$

If we set $p = 2$, we obtain a Hilbert space equipped with the inner product

$$(u,v)_{L^2(\Omega)} := \int_\Omega u(x)\overline{v(x)}\,\mathrm{d}x, \quad \text{for } \ u,v \in L^2(\Omega).$$

The local space $L^p_{\mathrm{loc}}(\Omega)$ contains all measurable functions u satisfying $u|_K \in L^p(K)$ for every measurable set K that is compactly embedded in Ω.

A function $v \in L^2(\Omega)$ is called j-th weak partial derivative of $u \in L^2(\Omega)$ if it satisfies

$$(\varphi, v)_{L^2(\Omega)} = (-1)^{|j|}(\partial^j\varphi, u)_{L^2(\Omega)} \quad \text{for all } \varphi \in C_c^\infty(\Omega),$$

where j is a multi-index and ∂^j is the differential operator defined in (2.1), see [GT77, Sec. 7.3]. If the weak derivative exists, we write $\partial^j u = v$. In the theory of partial differential equations, the L^2-based Sobolev spaces

$$H^k(\Omega) := \{u \in L^2(\Omega) \mid \text{there exists } v \in L^2(\Omega) \text{ such that } \partial^j u = v \text{ for all } j \in \mathbb{N}_0^d \text{ with } |j| \leq k\}$$

for $k \in \mathbb{N}$, play an important role. Equipped with the inner product

$$(u,v)_{H^k(\Omega)} := \sum_{|j|\leq k} (\partial^j u, \partial^j v)_{L^2(\Omega)}$$

they form Hilbert spaces. Furthermore, the local Sobolev spaces $H^k_{\mathrm{loc}}(\Omega)$, $k \in \mathbb{N}$ are relevant for a variational formulation of a scattering problem in an unbounded domain, which are defined analogously to the local Lebesgue spaces. The fractional Sobolev spaces $H^s(\Omega)$, $s \in \mathbb{R}_{\geq 0}$, are the spaces containing all functions $u \in H^k(\Omega)$, where $s = k + \mu$, $0 < \mu < 1$, such that

$$\iint_\Omega \frac{|\partial^j u(x) - \partial^j u(y)|^2}{|x-y|^{d+2\mu}} < \infty.$$

For a reasonable formulation of boundary conditions, it is essential to impose certain requirements on the regularity of the boundary. Since the boundary of a domain is a manifold of dimension $d-1$ and thus has a Lebesgue measure zero, it must be clarified how a function from a Sobolev space is defined on this manifold.

Referring to [KH15, Def. 5.1], the boundary $\partial\Omega$ of a domain Ω is said to be C^k smooth if it can be parameterized locally by C^k functions. We assume there exists a finite number $J \in \mathbb{N}$ of open cylinders

$$U_j := \{R_j x + z^{(j)} \mid x \in B'_{r_j}(0) \times (-2\beta_j, 2\beta_j)\}, \quad j = 1, \dots, J,$$

with translation vectors $z^{(j)} \in \mathbb{R}^d$ and rotation matrices $R_j \in \mathbb{R}^{d\times d}$ and denote by $B'_{r_j}(0) := \{x' = (x_1, \dots, x_{d-1}) \in \mathbb{R}^{d-1} \mid |x'| \le r_j\} \subseteq \mathbb{R}^{d-1}$ the $d-1$ dimensional ball of radius r_j centered at the origin. In addition, we assume that there exist real-valued functions $\xi_j \in C^k(\overline{B'_{r_j}(0)})$ with $|\xi_j(x')| \le \beta_j$ for all $x' \in B'_{r_j}(0)$ such that $\partial\Omega \subset \bigcup_{j=1}^J U_j$ and

$$\begin{aligned} \partial\Omega \cap U_j &= \{R_j x + z^{(j)} \mid x' \in B'_{r_j}(0),\, x_d = \xi_j(x')\}\,, \\ \Omega \cap U_j &= \{R_j x + z^{(j)} \mid x' \in B'_{r_j}(0),\, x_d < \xi_j(x')\}\,, \\ U_j \backslash \overline{\Omega} &= \{R_j x + z^{(j)} \mid x' \in B'_{r_j}(0),\, x_d > \xi_j(x')\}\,. \end{aligned}$$

If the functions ξ_i lie in $C^{k,\alpha}(\overline{B'_{r_j}(0)})$, we say that $\partial\Omega$ is $C^{k,\alpha}$ smooth. For Lipschitz-continuous functions $\xi_i \in C^{0,1}(\overline{B'_{r_j}(0)})$ we call the domain Ω Lipschitz-bounded. According to Rademacher's theorem, the Lipschitz-boundedness of Ω ensures that the local parameterizations

$$\phi_j(x') = R_j \begin{pmatrix} x' \\ \xi_j(x') \end{pmatrix} + z^{(j)}, \quad x' \in B'_{r_j}(0)$$

of $\partial\Omega$ are almost everywhere differentiable, see [Eva98, Sec. 5.8, Thm. 6]. Consequently, if Ω has a Lipschitz boundary, the outer unit normal $\nu(x)$ is defined at almost every point $x \in \partial\Omega$, see [KH15, A.8]. Using the local coordinate system $\{(U_j, \xi_j) \mid j = 1, \dots, J\}$ and a corresponding partition of unity $\lambda_j,\ j = 1, \dots J$ on $\partial\Omega$, the spaces $C^1(\partial\Omega)$ and $C^1_t(\partial\Omega)$ can be defined by

$$\begin{aligned} C^1(\partial\Omega) &:= \{u \in C(\partial\Omega) \mid (\lambda_j u) \circ \phi_j \in C^1(B'_{r_j}(0)) \text{ for } j = 1, \dots, J\}\,, \\ C^1_t(\partial\Omega) &:= \{F \in C(\partial\Omega, \mathbb{C}^d) \mid F_k \in C^1(\partial\Omega), k = 1, \dots, d \text{ and } F \cdot \nu = 0 \text{ on } \partial\Omega\}\,, \end{aligned}$$

see [KH15, A.14].

For $u \in C^1(\overline{\Omega})$, the restriction of u to the boundary $\partial\Omega$ is called the trace of u. We introduce the trace operator, which is well-defined, by

$$\gamma_0 \colon C^1(\overline{\Omega}) \to C(\partial\Omega), \quad \gamma_0 u = u|_{\partial\Omega}\,. \tag{2.2}$$

According to [Mon03, Thm. 3.9], the trace operator γ_0 can be extended to a bounded operator from $H^1(\Omega)$ to $H^{\frac{1}{2}}(\partial\Omega)$, where we define the fractional Sobolev space $H^{\frac{1}{2}}$ by

$$H^{\frac{1}{2}}(\partial\Omega) := \{f \in L^2(\partial\Omega) \mid \text{there exists } u \in H^1(\Omega) \text{ such that } f = u|_{\partial\Omega}\}\,.$$

Furthermore, the $H^{\frac{1}{2}}$-norm is given by

$$\|f\|_{H^{\frac{1}{2}}(\partial\Omega)} := \inf\{\|u\|_{H^1(\Omega)} \mid u \in H^1(\Omega) \text{ with } \gamma_0 u = f\}$$

and we denote by $H^{-\frac{1}{2}}(\partial\Omega)$ the dual space of $H^{\frac{1}{2}}(\partial\Omega)$. If Ω belongs to the class $C^{0,1}$, the trace operator γ_0 is a continuous operator from $H^s(\Omega)$ to $H^{s-\frac{1}{2}}(\partial\Omega)$ for $s \in (\frac{1}{2}, 1]$ and has a right continuous inverse. The same statement is true for $s \in (\frac{1}{2}, k]$ if Ω is a $C^{k-1,1}$ domain, see [McL00, Thm. 3.37]. The space $H^s(\partial\Omega),\ s > \frac{1}{2}$ can therefore be defined by

$$H^s(\partial\Omega) := \{f \in L^2(\partial\Omega) \mid \text{there exists } u \in H^{s+\frac{1}{2}}(\Omega) \text{ such that } f = u|_{\partial\Omega}\}.$$

Let $\nu \in \mathbb{R}^d$ be the unit outward normal vector to a domain Ω of class $C^{1,1}$. The Neumann trace operator, which assigns to a function the normal component of its gradient on the boundary, is given by

$$\gamma_1 \colon C^1(\Omega) \to C(\partial\Omega), \quad \gamma_1 u = \left.\frac{\partial u}{\partial \nu}\right|_{\partial\Omega}. \tag{2.3}$$

With the definition of the trace operator γ_0, we obtain for $u \in H^2(\Omega)$ that $u \mapsto \partial u/\partial\nu$ is a linear continuous mapping from $H^2(\Omega)$ to $H^{\frac{1}{2}}(\partial\Omega)$, where the normal derivative at the boundary is specified by $(\partial u/\partial\nu)|_{\partial\Omega} = \nu \cdot \gamma_0(\nabla u)$. Moreover, this mapping can be extended to a bounded and well-defined operator from the space

$$H_D := \left\{u \in H^1(\Omega) \;\middle|\; \int_\Omega \left[\nabla u \cdot \nabla\varphi - k^2 u\varphi\right] \mathrm{d}x = 0 \text{ for all } \varphi \in H_0^1(\Omega)\right\}$$

of the variational solutions of the Helmholtz equation into $H^{-\frac{1}{2}}(\partial\Omega)$, see [KH15, Def. 5.17]. Note that $H_0^1(\Omega)$ refers to the space with vanishing trace, i.e., $u \in H^1(\Omega)$ with $\gamma_0 u = 0$.

2.2. Model Settings

We continue with a brief introduction to the physical background of time-harmonic acoustic wave scattering by impermeable thin-coated obstacles. This section is a short summary based on the works [CK13, Né01], where more detailed explanations can be found.

The acoustic wave equation describes the propagation of sound in a medium, which in our case is assumed to be homogeneous. The scalar wave equation for an isotropic pressure p is given by

$$\frac{1}{c_0^2}\frac{\partial^2 p(x,t)}{\partial t^2} - \Delta_x p(x,t) = 0, \quad x \in \mathbb{R}^3,\ t > 0, \tag{2.4}$$

whereby c_0 is the speed of sound in the medium. According to the linearized Euler equation, there exists a velocity potential $U = U(x,t)$ that fulfills equation (2.4). Considering time-harmonic acoustic waves of the form

$$U(x,t) = \mathrm{Re}\left(u(x)\mathrm{e}^{-\mathrm{i}\omega t}\right)$$

for a time frequency $\omega > 0$ and a complex-valued amplitude u, the wave equation reduces to the

Helmholtz equation

$$\Delta u(x) + k^2 u(x) = 0,$$

where the wave number k is given by the positive constant $k := \omega/c_0$.

In the following, we are interested in the scattering of time-harmonic waves at an obstacle D, modeled by a boundary value problem for the Helmholtz equation. Let D be a bounded domain in $\mathbb{R}^d$, $d \in \{2, 3\}$, with a Lipschitz continuous boundary ∂D. If an incident plane wave $u^i(x) = \mathrm{e}^{\mathrm{i}k\theta\cdot x}$ with propagation direction $\theta \in S^{d-1}$ and real positive wave number k that satisfies the Helmholtz equation

$$\Delta u^i + k^2 u^i = 0 \quad \text{in } \mathbb{R}^d$$

is scattered by the object D, this generates the scattered wave u^s. The superposition of these waves $u = u^i + u^s$, which is called the total field, is a solution to the Helmholtz equation

$$\Delta u + k^2 u = 0 \quad \text{in } \mathbb{R}^d \backslash \overline{D}. \tag{2.5}$$

The mathematical description of the scattering of time-harmonic waves at a bounded obstacle leads to a boundary value problem for the Helmholtz equation, whereby we still have to specify which condition should be fulfilled on the boundary of the scattering object. For example, in the case of acoustic scattering by a sound-soft obstacle, the total pressure at the boundary disappears (Dirichlet condition), whereas in the case of acoustic scattering by a sound-hard obstacle, the normal component of the velocity of the total field vanishes at the boundary (Neumann condition). Moreover, the classical impedance boundary condition arises when the normal velocity at the boundary is proportional to the excess pressure at the boundary, i.e.,

$$\frac{\partial u}{\partial \nu} + \lambda u = 0 \quad \text{on } \partial D.$$

The acoustic impedance of the obstacle is given here by $\lambda = \mathrm{i}\chi\rho\omega$, where ρ is the density, ω the frequency, and χ the proportionality coefficient, see [Col84].

To model more complex material surfaces with greater accuracy, generalized impedance boundary conditions with second-order (or higher) tangential derivatives are considered. In some literature, the term Ventcel boundary condition ([BNDHV10]) or more generally, effective boundary condition ([SV95, BL96]) is used instead of generalized impedance boundary condition.

In this thesis, we focus on a particular class of nonlinear generalized impedance boundary conditions, but before specifying them in more detail, we impose a condition on the scattered field at infinity to complete the formulation of the scattering problem.

The scattered field u^s is assumed to satisfy the Sommerfeld radiation condition (SRC)

$$\lim_{r\to\infty} r^{\frac{d-1}{2}} \left(\frac{\partial u^s(x)}{\partial r} - \mathrm{i}ku^s(x) \right) = 0, \quad r = |x|, \tag{2.6}$$

uniformly with respect to $\hat{x} = x/|x|$. This radiation condition prescribes the asymptotic behavior of solutions to the scattering problem in the exterior domain to ensure the uniqueness of the solution. In physical terms, this condition means that $u^s(x)e^{-\mathrm{i}\omega t}$ must be an outgoing wave, hence, no energy may be radiated in from infinity, [Col84].

2.2.1. Nonlinear Generalized Impedance Boundary Conditions

When mathematically describing the scattering of acoustic waves by a fully or partially penetrable inhomogeneity, for example, by a highly absorbent material or by a perfect conductor covered with a dielectric, challenges may arise. On the one hand, the behavior of the wave inside the inhomogeneity and on the other hand outside the inhomogeneity would have to be taken into account. To avoid such a problem, the idea is to replace the exact model inside the inhomogeneity by a generalized impedance boundary condition (GIBC), see, e.g., [BL96, HJ02]. The advantage of using such approximate models is that the small-scale phenomena do not need to be taken into account, which significantly simplifies the numerical implementation of the scattering problem.

We will now take a closer look at the example of a perfectly conducting obstacle covered by a thin layer of nonlinear material. For the notation of the required differential geometric bases, we follow the work of Nédélec, see [Né01, Sec. 2.5.6]. For further examples of the use of generalized impedance boundary conditions in scattering theory, we refer to [HJNS05, DHJ06, Cha12].

Let ν denote the unit normal vector to ∂D oriented towards $\mathbb{R}^d \backslash \overline{D}$. Throughout this section, we assume that the boundary ∂D is of class C^k for $k \geq 1$. Thus, there exists a sufficiently small $\epsilon_0 \in \mathbb{R}$ and a tubular neighborhood $\mathcal{U}_\epsilon \subset \mathbb{R}^d$ of ∂D, such that

$$\partial D \times [-\epsilon_0, \epsilon_0] \to \mathcal{U}_\epsilon, \quad (x, \epsilon) \mapsto x_\epsilon = x + \epsilon \nu(x)$$

is a C^{k-1} diffeomorphism. For any function f defined on ∂D, we assign the function $\widetilde{f}$ defined on the tubular neighborhood $\mathcal{U}_\epsilon$ to

$$\widetilde{f}(x_\epsilon) = f(\mathcal{P}(x_\epsilon)) = f(x),$$

where $\mathcal{P}(x_\epsilon)$ is the unique projection of x_ϵ onto the surface ∂D. The following definition can be found, for example, in [KH15, Def. A16].

Definition 2.1. (i) The surface gradient of $f \in C^1(\partial D)$ is defined as the orthogonal projection of $\nabla \widetilde{f}$ into the tangential plane, i.e.,

$$\nabla_\tau f := \nu \times (\nabla \widetilde{f} \times \nu) = \nabla \widetilde{f} - \frac{\partial \widetilde{f}}{\partial \nu} \nu \quad \text{on } \partial D.$$

(ii) Let $F \in C^1_t(\partial D)$ be a tangential vector field with extension $\widetilde{F} \in C^1(\mathcal{U}_\epsilon, \mathbb{C}^d)$. Then the surface divergence of F is given by

$$\operatorname{Div}(F) := \operatorname{div}(\widetilde{F}) - \nu \cdot (\widetilde{F}' \nu) \quad \text{on } \partial D,$$

where $\widetilde{F}' \in \mathbb{C}^{d \times d}$ is the Jacobian matrix of $\widetilde{F}$.

The following example motivates the derivation of an effective boundary condition for the special case of a two-dimensional perfectly conducting object, covered by an inhomogeneous thin film exhibiting a Kerr-type nonlinearity. Effective boundary conditions, which provide a formal description of (linear) thin-film approximations through an asymptotic expansion, have been investigated several times in recent years, see, e.g., [AHŞ11, AA96, AH98]. A generalization to

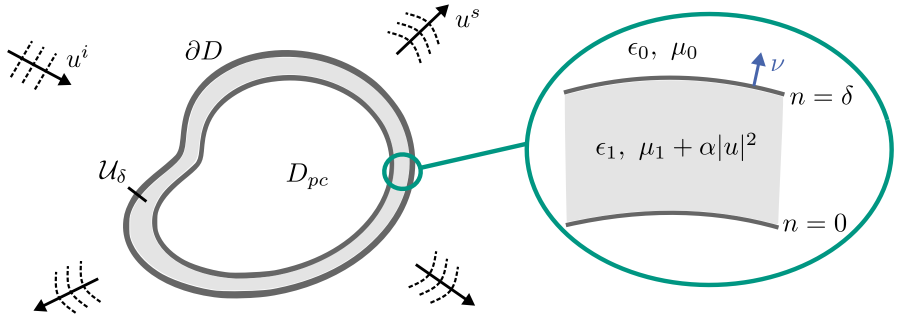

Figure 2.1. Scattering object coated with an inhomogeneous thin film containing a Kerr-type nonlinearity.

nonlinear coatings of ferromagnetic type in the scattering of electromagnetic waves has been shown by Haddar and Joly in [HJ02]. Furthermore, Norgren and He have considered the scattering on a plane metallic surface that is covered with an inhomogeneous nonlinear thin film, see [NH99]. For this, they assumed sound-soft boundary conditions (Dirichlet data), whereas we are interested in the case of sound-hard boundary conditions (Neumann data) at the boundary of the scattering object.

Example 2.2. In this example, we examine the scattering of electromagnetic waves in $\mathbb{R}^2$. For simplicity, we only consider incident waves that are polarized parallel to the axis of a cylinder representing the scatterer, and the magnetic field has only one component in the direction of the cylinder axis. This is referred to as the transverse electric mode or TE mode in scattering theory.

We denote the perfectly conductive scattered object by D_{pc} with a sufficiently smooth boundary curve $\Gamma \subseteq \partial D_{pc}$, the thin layer by $\mathcal{U}_\delta$, and the entire object by $D = \overline{D_{pc}} \cup \mathcal{U}_\delta$. In the case of a TE-polarized incident electromagnetic field, the total magnetic field has the form $H(x) = u(x_1, x_2)e_3$, where e_3 is the unit vector along the x_3 direction. The Maxwell equations are then reduced to

$$\operatorname{div}\left(\frac{1}{\epsilon_1}\nabla u\right) + \omega^2\left[\mu_1 + \alpha|u|^2\right]u = 0 \quad \text{in } \mathcal{U}_\delta,$$

see [AA96]. Here, ϵ_1 is the constant permittivity and $\mu_1 + \alpha|u|^2$ the permeability inside the layer. The frequency of the wave is represented by ω. In the exterior region of the layer, there is a vacuum with constant permittivity ϵ_0 and constant permeability μ_0.

At the boundary of the perfectly conducting object, i.e., at $n = 0$, the Neumann boundary condition

$$\frac{\partial u}{\partial \nu} = 0 \quad \text{on } \partial D_{pc}$$

is satisfied, and on the boundary curve $\Gamma_\delta \subseteq \partial D$, the relations

$$\frac{1}{\epsilon_1}\,\partial_\nu u\big|_{n=\delta^-} = \frac{1}{\epsilon_0}\,\partial_\nu u\big|_{n=\delta^+} \quad \text{and} \quad u|_{n=\delta^-} = u|_{n=\delta^+}$$

are valid. Note that δ^- refers to the inner trace on the boundary ∂D, i.e., $n \to \delta$ for $n \in (0,\delta)$ and δ^+ to the outer trace on ∂D, i.e., $n \to \delta$ for $n \in (\delta, \infty)$.

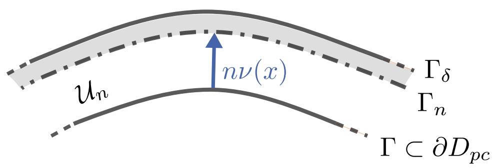

FIGURE 2.2. Thin layer on the surface of a perfectly conducting obstacle.

In the exterior domain, u solves the Helmholtz equation

$$\Delta u + k^2 u = 0 \quad \text{in } \mathbb{R}^2 \backslash \overline{D}$$

and $u - u^i$ satisfies the Sommerfeld radiation condition (2.6).

The parameterization of the neighbourhood of $\Gamma \subseteq \partial D$ is indicated by (s, n). Here, the variable s describes the tangential coordinate of x and the variable n is the distance $n = |x_n - x|$, where $x \in \Gamma$ is the orthogonal projection of a point x_n onto Γ, see Figure 2.2. The boundary curve Γ_n of the thin layer $\mathcal{U}_n$ is then defined by

$$\Gamma_n = \{x_n = x + n\nu(x)\}\,.$$

Furthermore, the curvature of Γ_n at a point (s, n) is denoted by $\kappa(s, n)$.

Inside the thin layer, we can asymptotically expand $u(s, n; \delta)$ in the following form

$$u(s, n; \delta) = u^{(0)}(s, \tau) + \delta u^{(1)}(s, \tau) + \delta^2 u^{(2)}(s, \tau) + \dots, \tag{2.7}$$

where the variable τ is given by $\tau = n/\delta$. The curvature $\kappa(s, n)$ can be expanded as

$$\kappa(s, \delta\tau) = \kappa(s, 0) + \delta\tau\kappa'(s, 0) + \dots, \tag{2.8}$$

where $\kappa'(s, 0) = \partial_n \kappa(s, n)|_{n=0}$. At the surface $n = \delta^+$ we have

$$u|_{n=\delta^+} = u^{(0)}|_{\tau=1} + \delta u^{(1)}|_{\tau=1} + \delta^2 u^{(2)}|_{\tau=1} + \delta^3 u^{(3)}|_{\tau=1} + \dots, \tag{2.9}$$

$$\partial_n u|_{n=\delta^+} = \frac{\epsilon_0}{\epsilon_1} \partial_n u|_{n=\delta^-} = \frac{\epsilon_0}{\epsilon_1 \delta} \left[\partial_\tau u^{(0)}|_{\tau=1} + \delta \partial_\tau u^{(1)}|_{\tau=1} + \delta^2 \partial_\tau u^{(2)}|_{\tau=1} + \dots \right], \tag{2.10}$$

see, e.g., [AH98]. If we insert the asymptotic expansion of u into the Helmholtz equation and rearrange the coefficients of $\delta^{-2}, \delta^{-1}, \delta^0$ and δ^1, we obtain four equations by equating the powers of δ. Integrating these equations with respect to τ and evaluating at $\tau = 1$ yields the approximated second-order impedance boundary condition

$$\begin{aligned} \partial_n u + \omega^2 \epsilon_1 \delta \left[\tilde{\mu}_1 - \delta\kappa(s, 0) \tilde{\tilde{\mu}}_1 \right] u - \partial_s \left(\left[\frac{1}{2} \delta^2 \kappa(s, 0) - \delta \right] \partial_s u \right) + \delta^2 \kappa(s, 0) \partial_s^2 u \\ = \omega^2 \epsilon_1 \delta \left[\delta\kappa(s, 0) \tilde{\tilde{\alpha}} - \tilde{\alpha} \right] |u|^2 u \end{aligned}$$

on the surface $n = \delta^+$, where

$$\tilde{\mu}_1(s) = \int_0^1 \mu_1(s,\tau)\,\mathrm{d}\tau \quad \text{and} \quad \tilde{\tilde{\mu}}_1(s) = \int_0^1 \int_0^\tau \mu_1(s,\tau_1)\,\mathrm{d}\tau_1\,\mathrm{d}\tau,$$
$$\tilde{\alpha}(s) = \int_0^1 \alpha(s,\tau)\,\mathrm{d}\tau \quad \text{and} \quad \tilde{\tilde{\alpha}}(s) \quad = \int_0^1 \int_0^\tau \alpha(s,\tau_1)\,\mathrm{d}\tau_1\,\mathrm{d}\tau.$$

A more detailed explanation of the calculation steps can be found in Appendix A. △

This example gives a small glimpse into what a nonlinear impedance boundary condition can look like. Throughout this thesis, we consider boundary conditions of the form

$$\frac{\partial u}{\partial \nu} + \mathrm{i}k\Big(\lambda u - \mathrm{Div}\,(\mu \nabla_\tau u)\Big) = g(\cdot, u) \quad \text{on} \quad \partial D, \tag{2.11}$$

where ν denotes the unit normal vector to ∂D oriented towards $\mathbb{R}^d \backslash \overline{D}$, $\lambda, \mu \in L^\infty(\partial D)$ are complex-valued impedance functions and $g\colon \partial D \times \mathbb{C} \to \mathbb{C}$ gives an additional nonlinear term with respect to u.

The direct scattering problem under consideration, therefore, consists of finding the total wave $u = u^i + u^s$ such that

$$\text{(SP)} \quad \begin{cases} \Delta u + k^2 u = 0 & \text{in } \mathbb{R}^d \backslash \overline{D}, \\ \dfrac{\partial u}{\partial \nu} + \mathrm{i}k\Big(\lambda u - \mathrm{Div}\,(\mu \nabla_\tau u)\Big) = g(\cdot, u) & \text{on } \partial D, \\ \lim\limits_{r \to \infty} r^{\frac{d-1}{2}} \left(\dfrac{\partial u^s(x)}{\partial r} - \mathrm{i}k u^s(x) \right) = 0, & r = |x|. \end{cases}$$

For the analytical examination of the problem regarding the existence and uniqueness in an appropriate function space, we consider a variational formulation of (SP).

2.3. Variational Formulation

In the given scattering problem (SP), the propagation region of the wave is unbounded. For the corresponding variational formulation, we consider an equivalent representation of the problem on a bounded subdomain. For this purpose, we place a ball $B_R(0) := \{x \in \mathbb{R}^d : |x| < R\}$ with radius $R > 0$ centered at the origin around the scattering obstacle D, such that it is fully contained in $B_R(0)$, i.e., $\overline{D} \subset B_R(0)$. Hence, the bounded subdomain of interest is given by $\Omega_R := B_R(0) \backslash \overline{D}$. From now on, we use the shorter notation B_R instead of $B_R(0)$.

Let ∂D be of class $C^{1,1}$. The generalized impedance boundary condition contains second-order derivatives on ∂D. Consequently, the $H^{\frac{1}{2}}-$regularity on the boundary, by applying the trace on $H^1_{\mathrm{loc}}(\mathbb{R}^d \backslash \overline{D})$, is not sufficient for a suitable variational formulation of the scattering problem. Therefore, we introduce the Sobolev space

$$V_R = \{v \in H^1(\Omega_R) \mid v|_{\partial D} \in H^1(\partial D)\}\,.$$

Equipped with the inner product

$$(\cdot,\cdot)_{V_R} = (\cdot,\cdot)_{H^1(\Omega_R)} + (\cdot,\cdot)_{H^1(\partial D)}\,,$$

the space V_R is a Hilbert space, see [KCDQ15].

To include the Sommerfeld radiation condition, we specify a nonlocal boundary condition on ∂B_R, which ensures a unique continuation of the solution in $\mathbb{R}^d \backslash \overline{D}$. Therefore, we introduce the Dirichlet-to-Neumann map

$$\Lambda \colon H^{\frac{1}{2}}(\partial B_R) \to H^{-\frac{1}{2}}(\partial B_R), \quad \Lambda f = \frac{\partial w}{\partial \nu}\,,$$

where w is the radiating solution of the Helmholtz equation outside the ball B_R, with Dirichlet trace $w = f$ on ∂B_R. Here, a radiating solution refers to a solution of the previously mentioned problem, which satisfies the Sommerfeld radiation condition (2.6). Using the Dirichlet-to-Neumann operator Λ provides an equivalent formulation of the scattering problem (2.5)–(2.6) on a bounded domain:

Find $u \in V_R$ such that

$$\text{(SP)} \quad \begin{cases} \Delta u + k^2 u = 0 & \text{in } \Omega_R, \\ \dfrac{\partial u}{\partial \nu} + \mathrm{i}k\Big(\lambda u - \mathrm{Div}\,(\mu \nabla_\tau u)\Big) = g(\cdot, u) & \text{on } \partial D, \\ \dfrac{\partial u}{\partial \nu} - \Lambda u = \dfrac{\partial u^i}{\partial \nu} - \Lambda u^i & \text{on } \partial B_R. \end{cases}$$

A variational formulation of the scattering problem is then given by

$$\mathcal{R}(u,v) = (f,v)_{V_R} \quad \text{for all } v \in V_R \tag{2.12}$$

with

$$\begin{aligned} \mathcal{R}(u,v) = &\int_{\Omega_R} \nabla u \cdot \nabla \overline{v} - k^2 u \overline{v} \,\mathrm{d}x - \mathrm{i}k \int_{\partial D} \lambda u \overline{v} \,\mathrm{d}s - \mathrm{i}k \int_{\partial D} \mu \nabla_\tau u \cdot \nabla_\tau \overline{v} \,\mathrm{d}s \\ &+ \int_{\partial D} g(\cdot, u) \overline{v} \,\mathrm{d}s - \int_{\partial B_R} \Lambda u \overline{v} \,\mathrm{d}s\,, \end{aligned}$$

and $f \in V_R$ is defined from the representation theorem by

$$(f,v)_{V_R} = \int_{\partial B_R} \left(\frac{\partial u^i}{\partial \nu} - \Lambda u^i \right) \overline{v} \,\mathrm{d}s\,. \tag{2.13}$$

To ensure that the integral over the nonlinear function g is reasonable, we assume throughout this work that $g(x,z)$ is measurable in x, continuous in z, and satisfies the growth condition

$$|g(x,z)| \le |\psi(x)| + c|z|^p \quad \text{for a.e. } x \in \partial D,\ z \in \mathbb{C}, \tag{2.14}$$

with $c > 0$, $\psi \in L^2(\partial D)$ and $1 \le p < \infty$.

Remark 2.3. The growth condition (2.14) is commonly restricted to $1 \leq p \leq 2$ for $d = 3$ to ensure that $g(x,u) \in L^2(\partial D)$ when only $u \in H^1(\Omega_R)$ is assumed, which stems from the Sobolev embedding $H^{1/2}(\partial D) \hookrightarrow L^q(\partial D)$ for $q \leq 4$. In the present setting, however, the additional boundary regularity $u|_{\partial D} \in H^1(\partial D)$ implies $u|_{\partial D} \in L^q(\partial D)$ for all $q < \infty$, and in particular $u \in L^{2p}(\partial D)$ for all $p < \infty$. As a result, the condition $1 \leq p < \infty$ is sufficient even in three dimensions. ♢

Then the image of the Nemytskii operator $G\colon V_R \to L^2(\partial D)$, $G(u)(x) = g(x,u(x))$ belongs to $L^2(\partial D)$ for all $u \in V_R$, and

$$\|G(u)\|_{L^2(\partial D)} \leq c\Big(\|\psi\|_{L^2(\partial D)} + \|u\|_{V_R}^p\Big)$$

for a constant $c > 0$, see [AF03, Thm. 5.36] and [Sho97, Thm. 3.2]. Functions with these properties are often referred to in the literature as Carathéodory functions. Further conditions on g will be specified below.

2.3.1. Well-posedness in H^1_{loc}

According to Hadamard, a problem is well-posed if it has a unique solution that depends continuously on the data. The last condition means that for a given operator equation $A(u) = f$, the inverse operator A^{-1} is continuous. For the nonlinear case, however, we only require boundedness of A^{-1}, which is sufficient for all subsequent considerations in this thesis. It is well known for the linear scattering problem, i.e., $g \equiv 0$, that there exists a unique solution $u \in V_R$ of (2.12) for any $f \in V_R$, if the impedance functions satisfy $\mathrm{Re}(\lambda) \geq 0$ and $\mathrm{Re}(\mu) \geq 0$, see [Kre18, Kre19]. Thus, throughout this work, we assume $\mathrm{Re}(\lambda) \geq 0$ and $\mathrm{Re}(\mu) \geq 0$ on ∂D. In order to ensure a well-posed direct boundary value problem even in the case of the nonlinear boundary condition, we exploit the fact that the uniqueness of a solution to the linear equation implies the existence of a solution to the nonlinear equation. The following theorem by Kačurovskii from 1970 is an extension of the linear Fredholm theory to integral equations or boundary value problems for semilinear elliptic equations, see [ZB90, Thm. 29.A].

Theorem 2.4 (Kačurovskii)**.** *We consider the nonlinear operator equation*

$$u + Lu + N(u) = b, \quad u \in X, \tag{2.15}$$

and suppose that the operators $L, N\colon X \to X$ are compact on the Banach space X. Furthermore, we assume that L is linear and $L + N$ is asymptotically linear , i.e.,

$$\frac{\|N(u)\|}{\|u\|} \to 0 \quad \text{as} \quad \|u\| \to \infty.$$

Then:

(i) *If $(I + L)u = 0$ implies $u = 0$, then equation* (2.15) *has a solution for each $b \in X$.*

(ii) *If $\mathcal{R}(N) \subseteq \mathcal{R}(I + L)$, then equation* (2.15) *has a solution u if and only if $b \in \mathcal{R}(I + L)$.*

The statement (i) claims that if the linear equation $u + Lu = b$ has at most one solution u, then the nonlinear equation $u + Lu + N(u) = b$ has a solution u. In other words, the uniqueness of a solution to the linear problem implies the existence of a solution to the nonlinear problem.

An operator is called a Fredholm operator of index zero if it is a compact perturbation of an invertible operator. Since L is compact by assumption, $(I + L)$ is Fredholm of index zero. Therefore, $\mathcal{R}(N) \subseteq \mathcal{R}(I + L)$ if and only if

$$\langle u^*, N(v)\rangle = 0 \quad \text{for all} \;\; u^* \in \mathcal{N}(I + L^*),\; v \in X.$$

Furthermore, $b \in \mathcal{R}(I + L)$ exactly when

$$\langle u^*, b\rangle = 0 \quad \text{for all} \;\; u^* \in \mathcal{N}(I + L^*),$$

see [ZB90, p. 651].

The proof of Kačurovskii's theorem is based on the Leray-Schauer fixed point index ([Zei86, Sec. 12.7, Thm. 12.B]), which we can apply after showing that the mappings $u \mapsto -Lu$ and $u \mapsto -Lu - (N(u) - b)$ are compactly homotopic. The mappings are called homotopic if there exists a continuous map $H\colon X \times [0, 1] \to X$ such that

$$H(u, 0) = -Lu \quad \text{and} \quad H(u, 1) = -Lu - (N(u) - b)\,.$$

In other words, $-Lu$ is deformed into $-Lu - (N(u) - b)$ on the time interval $[0, 1]$. At time t, the deformation is given by

$$H(x, t) = -Lu - t(N(u) - b)\,.$$

Let $\mathcal{U} = \{u \in X \mid \|u\| < R\}$. For sufficiently large R, we have the relation

$$H(u, t) \neq u \quad \text{for all } (u, t) \in \partial\mathcal{U} \times [0, 1]\,.$$

According to the existence principle (A2) in [Zei86, Def. 12.3], it can be shown that the equation $u = H(u, 1)$ for $u \in \mathcal{U}$ has a solution, i.e., $u + Lu + N(u) - b = 0$. For more details, see [Zei86, Sec. 12.2, Sec. 12.3] and [ZB90, Sec. 29.2].

Kačurovskii's theorem gives a sufficient condition for the existence of weak solutions to the scattering problem under consideration, provided that the function $g\colon \partial D \times \mathbb{C} \to \mathbb{C}$ satisfies an additional assumption.

Theorem 2.5 (Existence)**.** *Let the nonlinearity g be sublinear in z at infinity, i.e.,*

$$|g(x, z)| = o(|z|) \textit{ as } |z| \to \infty \quad \textit{for a.e. } x \in \partial D. \tag{2.16}$$

Then, for any $f \in V_R$, there exists a weak solution $u \in V_R$ of the boundary value problem (2.12)*.*

Proof. The variational formulation is equivalent to the operator equation

$$R_l u + R_n(u) = f \quad \text{in} \;\; V_R\,,$$

where the operators $R_l, R_n\colon V_R \to V_R^*$ are defined by

$$
\begin{aligned}
(R_l u, v)_{V_R} &= \int_{\Omega_R} \nabla u \cdot \nabla \overline{v} - k^2 u\overline{v} \,\mathrm{d}x - \mathrm{i}k \int_{\partial D} \lambda u \overline{v} \,\mathrm{d}s - \mathrm{i}k \int_{\partial D} \mu \nabla_\tau u \cdot \nabla_\tau \overline{v} \,\mathrm{d}s - \int_{\partial B_R} \Lambda u \overline{v} \,\mathrm{d}s\,, \\
(R_n(u), v)_{V_R} &= \int_{\partial D} g(\cdot, u)\overline{v} \,\mathrm{d}s\,.
\end{aligned} \tag{2.17}
$$

We identify $V_R \cong V_R^*$ via the Riesz isomorphism and consider R_l and R_n as mappings from V_R to V_R. The linear scattering problem is given by the operator R_l, which is an injective Fredholm operator of index zero that has a bounded inverse, see [BH10]. From

$$
\|R_n(w) - R_n(u)\|_{V_R} \leq \|G(w) - G(u)\|_{L^2(\partial D)}
$$

it follows that the operator R_n is continuous, since, due to the sublinear assumption, the Nemytskii operator G is continuous as a mapping from $L^2(\partial D)$ to $L^2(\partial D)$, see [Sho97, Cor. 3.4]. Moreover, the trace operator $\gamma\colon V_R \to L^2(\partial D),\ \gamma(u) = u|_{\partial D}$ is continuous and compact. Since the composition

$$
V_R \xrightarrow{\gamma} L^2(\partial D) \xrightarrow{G} L^2(\partial D) \xrightarrow{\gamma^*} V_R^*
$$

is continuous and γ is compact, the associated operator $R_n\colon V_R \to V_R$, obtained by composing γ, G, and γ^* and identifying V_R with its dual, is compact. By exploiting the continuity of the trace operator γ, we obtain

$$
|(R_n(u), v)_{V_R}| = \left| \int_{\partial D} g(\cdot, u)\,\overline{v}\ \mathrm{d}s \right| \leq \|g(\cdot, u)\|_{L^2(\partial D)} \|v\|_{L^2(\partial D)} \leq C \|g(\cdot, u)\|_{L^2(\partial D)} \|v\|_{V_R}\,,
$$

where the asymptotic behavior

$$
\|g(\cdot, u)\|_{L^2(\partial D)} = o\left(\|u\|_{L^2(\partial D)}\right) = o\Big(\|u\|_{V_R}\Big)
$$

follows from assumption (2.16). Thus, $R_l + R_n$ is asymptotically linear, since

$$
\frac{\|R_n(u)\|_{V_R}}{\|u\|_{V_R}} \leq \frac{C\|g(\cdot, u)\|_{L^2(\partial D)}}{\|u\|_{V_R}} \to 0 \quad \text{for } \|u\|_{V_R} \to \infty\,. \tag{2.18}
$$

Therefore, Kačurovskii's theorem can be applied, which ensures the existence of a solution to (2.12) for any $f \in V_R$. □

Now that we have established the existence of a solution, we will show that the scattering problem (2.12) has at most one solution. To prove the uniqueness using Rellich's lemma, we have to make a further assumption on g.

Let g be differentiable in its second argument in the sense that $g_z(\cdot, z; w) \in L^\infty(\partial D)$ exists, such that

$$
g(x, z + w) - g(x, z) = g_z(x, z; w) + o(|w|) \tag{2.19}
$$

for all $z, w \in \mathbb{C}$ and almost every $x \in \partial D$. Then a lower bound for $\mathrm{Re}(\lambda)$ and $\mathrm{Re}(\mu)$ leads to a unique solution of the direct scattering problem. Since g allows complex entries in its second component, we can only expect the linearization g_z to be $\mathbb{R}$-linear with respect to w and not

$\mathbb{C}$-linear. For a more detailed explanation of the notation of $g_z(x, z; w)$ and the $\mathbb{R}$-linearity with respect to w, please refer to Section 2.4.

Theorem 2.6 (Uniqueness). *Let $g\colon \partial D \times \mathbb{C} \to \mathbb{C}$ be a sublinear function as in Theorem 2.5, which is differentiable in its second argument in the sense of* (2.19)*. Furthermore let $\lambda, \mu \in L^\infty(\partial D)$ with $\mathrm{Re}(\mu) \geq 0$ and*

$$k\mathrm{Re}(\lambda) \geq \sup_{z,w\in\mathbb{C}} \frac{\mathrm{Im}(g_z(x, z; w)\overline{w})}{|w|^2} \quad \textit{for any } z, w \in \mathbb{C} \textit{ and a.e. } x \in \partial D.$$

Then, problem (2.12) *has a unique solution $u \in V_R$.*

Proof. Rellich's Lemma ensures that a radiating solution of the Helmholtz equation vanishes in $\mathbb{R}^d \backslash \overline{D}$ if

$$\int_{\partial D} \mathrm{Im}\left(\overline{u}\frac{\partial u}{\partial \nu}\right) \mathrm{d}s \leq 0,$$

see [CK13, Thm. 2.13]. Let u_1 and u_2 be two solutions of (2.12). We obtain the inequality for the scattered solution $u = u_1 - u_2$ of the Helmholtz equation, i.e.,

$$\begin{aligned}\int_{\partial D} \mathrm{Im}\left(\overline{u}\frac{\partial u}{\partial \nu}\right) \mathrm{d}s &= -k\int_{\partial D} \mathrm{Re}(\lambda)|u|^2 \,\mathrm{d}s - k\int_{\partial D} \mathrm{Re}(\mu)|\nabla_\tau u|^2 \,\mathrm{d}s \\ &\quad + \mathrm{Im}\int_{\partial D} \Big((g(\cdot, u_1) - g(\cdot, u_2))\overline{u}\Big) \,\mathrm{d}s \\ &\leq 0,\end{aligned}$$

where the inequality follows from the estimate

$$\mathrm{Im}\Big((g(x, z+w) - g(x, z))\overline{w}\Big) = \mathrm{Im}\int_0^1 g_z(x, z+tw; w)\overline{w} \,\mathrm{d}t \leq k\mathrm{Re}(\lambda)|w|^2 .$$

This implies uniqueness of the solution $u \in V_R$ to the scattering problem (2.12). ☐

Finally, for the scattering problem to be well-posed, we need to prove that it is stable with respect to small perturbations in the data.

Theorem 2.7 (Stability). *Let $g\colon \partial D \times \mathbb{C} \to \mathbb{C}$ be a sublinear function as in Theorem 2.5 and $u \in V_R$ be a solution of*

$$R_l u + R_n(u) = f \quad \textit{in } V_R\,,$$

where the linear operator R_l and the nonlinear operator R_n are defined as in (2.17)*.*

Then, for $\widetilde{C} > 0$, there exists a constant $C > 0$ such that

$$\|u\|_{V_R} \leq C \quad \textit{for any } f \in \left\{f \in V_R \mid \|f\|_{V_R} \leq \widetilde{C}\right\}. \tag{2.20}$$

Proof. In order to obtain the desired estimate, we must show that the operator $(R_l + R_n)^{-1}$ is bounded. We prove this statement by contradiction, namely, assuming that $(R_l + R_n)^{-1}$ is not bounded. Then, there exists a sequence $(f_n)_n \subset V_R$ with $\|f_n\|_{V_R} \leq \widetilde{C}$ for a constant $\widetilde{C} > 0$ and $\|(R_l + R_n)^{-1} f_n\|_{V_R} \to \infty$ for $n \to \infty$. We set $u_n = (R_l + R_n)^{-1} f_n$ and $z_n = u_n/\|u_n\|_{V_R}$. This implies that $\|z_n\| = 1$ and

$$R_l z_n = \frac{R_l u_n}{\|u_n\|_{V_R}} = \frac{(R_l + R_n)(u_n)}{\|u_n\|_{V_R}} - \frac{R_n(u_n)}{\|u_n\|_{V_R}} = \frac{f_n}{\|(R_l + R_n)^{-1} f_n\|_{V_R}} - \frac{R_n(u_n)}{\|u_n\|_{V_R}} \to 0 \quad \text{for } n \to \infty.$$

Here, we have utilized the asymptotic linearity of $R_l + R_n$ for the limit of the second term, see (2.18). Since R_n is compact, there exists a convergent subsequence $(z_{n_j}) = \left(u_{n_j}/\|u_{n_j}\|_{V_R}\right)$ with $\|z_{n_j}\|_{V_R} = 1$, for which

$$R_n(z_{n_j}) = R_n\left(\frac{u_{n_j}}{\|u_{n_j}\|}\right) \to v, \quad \text{for } j \to \infty,$$

is valid for some $v \in V_R$. This leads to

$$(R_l + R_n)(z_{n_j}) = R_l z_{n_j} + R_n(z_{n_j}) \to v, \quad \text{for } j \to \infty,$$

since $R_l z_{n_j} \to 0$ for $j \to \infty$. We know that the linear operator R_l is an injective Fredholm operator of index zero that has a bounded inverse. Hence, we have

$$z_{n_j} = R_l^{-1} R_l z_{n_j} = R_l^{-1}\left((R_l + R_n)(z_{n_j}) - R_n(z_{n_j})\right) \to R_l^{-1}(v - v) = 0 \quad \text{for } j \to \infty.$$

However, this contradicts $\|z_{n_j}\|_{V_R} = 1$. Therefore, the operator $(R_l + R_n)^{-1}$ is bounded and there exists a constant $C > 0$ such that

$$\|u\|_{V_R} = \|(R_l + R_n)^{-1} f\|_{V_R} \le C \quad \text{for any } f \in \left\{f \in V_R \mid \|f\|_{V_R} \le \widetilde{C}\right\}.$$

□

For our existence result, it is necessary that the nonlinear function $g(\cdot, z)$ grows sublinear with respect to z at infinity. This assumption may seem very restrictive, but numerical results show that the nonlinearity can be assumed to be negligible for large $|z|$, see Remark 2.8 (ii).

Remark 2.8. (i) As an example we may consider $g(\cdot, z) = z/(1 + |z|^2)$ under the assumption $k\mathrm{Re}(\lambda) \ge \frac{1}{2}$ on ∂D, where the linearization of g is given by

$$g_z(\cdot, z; w) = \frac{(1 + |z|^2)w - 2\mathrm{Re}(\overline{z}w)z}{(1 + |z|^2)^2},$$

see Example 2.10 (ii). Obviously, the function g is sublinear in z and with

$$\mathrm{Im}(g_z(\cdot, z; w)\overline{w}) = \mathrm{Im}\left(\frac{(1 + |z|^2)|w|^2 - 2\mathrm{Re}(\overline{z}w)z\overline{w}}{(1 + |z|^2)^2}\right) = -\frac{2\mathrm{Re}(z\overline{w})\,\mathrm{Im}(z\overline{w})}{(1 + |z|^2)^2}$$

and $|z|/(1 + |z|^2) \le 1/2$ for all $z \in \mathbb{C}$ we obtain the assumption of Theorem 2.6.

(ii) Note that the restriction of a sublinear function g is quite natural, since in the general well-posed case, g can be replaced by a sublinear function without changing the solution. This can be seen as follows: Let us assume that the boundary value problem (2.12) is well-posed, f is defined as in (2.13) by the incident field u^i, and $u = u^s + u^i$ denotes the solution of the scattering problem (SP). In addition, we assume that $\lambda \in C^1(\partial D)$ and $\mu \in C^2(\partial D)$ to ensure sufficient regularity. From Green's representation theorem for u^s in $\mathbb{R}^d \backslash \overline{D}$ and for u^i in D, ([CK13, Thm. 2.1, Thm. 2.3]), and the boundary condition (2.11) we obtain

$$\begin{aligned} u^s(x) - u^i(x) &= 2 \int_{\partial D} u(y) \frac{\partial \Phi(x,y)}{\partial \nu_y} + \Big(\mathrm{i}k\lambda u(y) - \mathrm{i}k \mathrm{Div}(\mu \nabla_\tau u(y)) - g(\cdot, u(y)) \Big) \Phi(x,y) \, \mathrm{d}s_y \\ &= 2\mathcal{D}u(x) + 2\mathcal{S}\Big(\mathrm{i}k\lambda u(x) - \mathrm{i}k \mathrm{Div}(\mu \nabla_\tau u(x)) - g(\cdot, u(x)) \Big) \end{aligned}$$

for $x \in \partial D$, where Φ is the fundamental solution of the Helmholtz equation and $\mathcal{S}, \mathcal{D}$ denote the boundary integral operators corresponding to the single-layer and the double-layer potential of the Helmholtz equation, see Section 2.4.1 and [KH15, Sec. 5.2].

For $D \subseteq \mathbb{R}^2$ with $\partial D \in C^{2,\alpha}$, $\alpha \in (0,1)$ we have $\mathcal{D}, \mathcal{S} \colon L^2(\partial D) \to H^1(\partial D) \subseteq C(\partial D)$, see [Kir89, Thm. 4.2 (b)]. Thus, for $u \in H^2(\partial D)$, the above representation holds pointwise and the Carathéodory condition (2.14) implies

$$\begin{aligned} \|u\|_{C(\partial D)} &\leq C\Big(\|u^i\|_{C(\partial D)} + \|u\|_{H^2(\partial D)} + \|\psi\|_{L^2(\partial D)} + \|u\|^p_{H^2(\partial D)} \Big) \\ &= b_0 \end{aligned}$$

for some $b_0 \in \mathbb{R}$. Analogously, this is true in the three dimensional case $D \subseteq \mathbb{R}^3$, provided that $\partial D \in C^{3,\alpha}$ and $g(\cdot, u) \in H^1(\partial D)$ for $u \in H^3(\partial D)$. In this case, $\mathrm{Div}(\mu \nabla_\tau u) \in H^1(\partial D)$ and the mapping properties of $\mathcal{D}, \mathcal{S} \colon H^1(\partial D) \to H^2(\partial D)$, see [Kir89, Thm. 4.3 (a)]), together with the Sobolev embedding $H^2(\partial D) \subseteq C(\partial D)$, yield the desired estimate.

Now consider g_b defined by $g_b(x,z) = \varphi_b(|z|) g(x,z)$ with $\varphi_b \in C^\infty(\mathbb{R})$ given by

$$\varphi_b(r) = \begin{cases} 1\,, & \text{for } r \leq b, \\ 0\,, & \text{for } r > b+1, \end{cases}$$

for $r \in \mathbb{R}$. We observe g_b to be sublinear in its second argument, and u solves the problem (2.12) for all $b > b_0$, if g is replaced by g_b. Thus, if g_b satisfies the conditions of Theorem 2.6 and u_b denotes the corresponding unique solution, we conclude $u = u_b$ for all $b > b_0$ by the uniqueness of the problem.

For the Kerr nonlinearity $g_b(\cdot, u) = \varphi_b(|u|)|u|^2 u$ with

$$\varphi_b(|z|) := \frac{\alpha\left((b+1)^2 - |z|^2\right)}{\alpha\left((b+1)^2 - |z|^2\right) + \alpha\left(|z|^2 - b^2\right)} \quad \text{and} \quad \alpha(x) = \begin{cases} \mathrm{e}^{-\frac{1}{x}}, & x > 0, \\ 0, & x \leq 0, \end{cases}$$

we can see numerically that for $b > b_0 = 1.2$ the solution u_b appears to be independent of b, see Figure 2.3. Here, the direct scattering problem was solved as described in Chapter 4. $\Diamond$

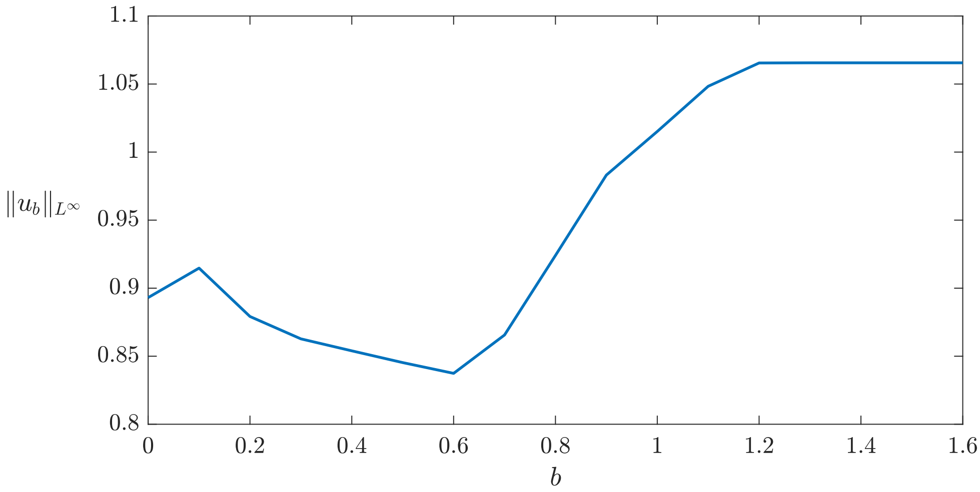

Figure 2.3. $L^\infty(\partial D)$−norm of the solution u_b to the scattering problem with nonlinearity $g_b(\cdot,u) = \varphi_b(|u|)|u|^2u$.

2.4. ℝ-linear Problem

For the first order expansion of the nonlinear function $g\colon \partial D \times \mathbb{C} \to \mathbb{C}$, we are dealing with the derivative of a scalar-valued function with complex parameters. We denote the pair of conjugate coordinates by

$$\mathbf{c} = (z, \overline{z})^\top \in \mathbb{C}^2$$

and $z = v + \mathrm{i}w$ with $v, w \in \mathbb{R}$. Furthermore, we extend the domain of the function g to $\partial D \times \mathbb{C} \times \mathbb{C}$ by treating z and its conjugate $\overline{z}$ as separate input variables. The notation

$$g(\cdot, \mathbf{c}) = g(\cdot, z, \overline{z}) = \widetilde{g}(\cdot, v, w) \in \mathbb{C}$$

can be used equivalently, where $\widetilde{g}$ is the corresponding function that maps from $\partial D \times \mathbb{R} \times \mathbb{R}$ to $\mathbb{C}$. Using this formulation of the function g, we can now specify the cogradient of g by fixing $\overline{z}$ and computing the partial derivative with respect to z, as well as the conjugate cogradient of g with the reverse order. These Wirtinger derivatives

$$\frac{\partial g(\cdot, z, \overline{z})}{\partial z}\bigg|_{\overline{z}\text{ const.}} \quad \text{and} \quad \frac{\partial g(\cdot, z, \overline{z})}{\partial \overline{z}}\bigg|_{z\text{ const.}} \tag{2.21}$$

are to be understood in the formal sense, since z and $\overline{z}$ are of course not independent of each other, see, e.g., [Rem91, Bra83].

Remark 2.9. Under the assumption that g is analytic with respect to z and $\overline{z}$ and that $\widetilde{g}\colon \partial D \times \mathbb{R} \times \mathbb{R} \to \mathbb{C}$ is the function of real variables v and w such that $g(\cdot, z, \overline{z}) = \widetilde{g}(\cdot, v, w)$, an equivalent representation of the derivatives (2.21) is expressed by

$$\frac{\partial g(\cdot, z, \overline{z})}{\partial z}\bigg|_{\overline{z}\text{ const.}} = \frac{1}{2}\left(\frac{\partial \widetilde{g}(\cdot, v, w)}{\partial v} - \mathrm{i}\frac{\partial \widetilde{g}(\cdot, v, w)}{\partial w}\right),$$

$$\frac{\partial g(\cdot,z,\overline{z})}{\partial \overline{z}}\bigg|_{z\text{ const.}} = \frac{1}{2}\left(\frac{\partial \widetilde{g}(\cdot,v,w)}{\partial v} + \mathrm{i}\frac{\partial \widetilde{g}(\cdot,v,w)}{\partial w}\right).$$

◊

The first order expansion in $\mathbf{c} \in \mathbb{C}\times\mathbb{C}$ is given by

$$\begin{aligned} g(\cdot,z+h,\overline{z}+\overline{h}) &= g(\cdot,z,\overline{z}) + \left(\frac{\partial g(\cdot,z,\overline{z})}{\partial z}\bigg|_{\overline{z}\text{ const.}}, \frac{\partial g(\cdot,z,\overline{z})}{\partial \overline{z}}\bigg|_{z\text{ const.}}\right)\cdot\begin{pmatrix} h \\ \overline{h}\end{pmatrix} + o(|h|) \\ &= g(\cdot,z,\overline{z}) + \frac{\partial g(\cdot,z,\overline{z})}{\partial z}\bigg|_{\overline{z}\text{ const.}} h + \frac{\partial g(\cdot,z,\overline{z})}{\partial \overline{z}}\bigg|_{z\text{ const.}} \overline{h} + o(|h|)\,. \end{aligned}$$

Throughout this thesis we use the shorter notation

$$g_z(\cdot,z;h) := \frac{\partial g(\cdot,z,\overline{z})}{\partial z}\bigg|_{\overline{z}\text{ const.}} h + \frac{\partial g(\cdot,z,\overline{z})}{\partial \overline{z}}\bigg|_{z\text{ const.}} \overline{h}\,. \tag{2.22}$$

The following example illustrates the calculation of the linearization g_z in the case of a cubic Kerr nonlinearity and the nonlinearity from Remark 2.8 (i).

Example 2.10. (i) For the cubic Kerr nonlinearity $g(\cdot,z) = |z|^2 z = z^2\overline{z}$, the cogradient and the conjugate cogradient of g are given by

$$\frac{\partial g(\cdot,z,\overline{z})}{\partial z}\bigg|_{\overline{z}\text{ const.}} = 2z\overline{z} \quad\text{and}\quad \frac{\partial g(\cdot,z,\overline{z})}{\partial \overline{z}}\bigg|_{z\text{ const.}} = z^2,$$

whereby we obtain

$$g_z(\cdot,z;h) = 2z\overline{z}h + z^2\overline{h} = |z|^2 h + 2\mathrm{Re}(\overline{z}h)z\,.$$

(ii) For the nonlinearity $g(\cdot,z) = z/(1+|z|^2)$ from Remark 2.8 (i) the cogradient and the conjugate cogradient are provided by

$$\frac{\partial g(\cdot,z,\overline{z})}{\partial z}\bigg|_{\overline{z}\text{ const.}} = \frac{1}{(1+|z|^2)^2} \quad\text{and}\quad \frac{\partial g(\cdot,z,\overline{z})}{\partial \overline{z}}\bigg|_{z\text{ const.}} = \frac{-z^2}{(1+|z|^2)^2}\,.$$

Therefore, we obtain

$$g_z(\cdot,z;h) = \frac{h - z^2\overline{h}}{(1+|z|^2)^2} = \frac{h + |z|^2h - |z|^2h - z^2\overline{h}}{(1+|z|^2)^2} = \frac{(1+|z|^2)h - 2\mathrm{Re}(\overline{z}h)z}{(1+|z|^2)^2}\,.$$

△

The representation (2.22) shows that we cannot expect the function g_z to be $\mathbb{C}$-linear with respect to h, since the homogeneity condition $g_z(\cdot,z;\lambda h) = \lambda g_z(\cdot,z;h)$ for $\lambda\in\mathbb{C}$ is not necessarily fulfilled. However, if we restrict the constant λ to the real line, then the homogeneity condition holds true. Therefore, the function g_z is $\mathbb{R}$-linear with respect to h, i.e.,

$$g_z(\cdot,z;h_1+h_2) = g_z(\cdot,z;h_1) + g_z(\cdot,z;h_2) \quad\text{and}\quad g_z(\cdot,z;\lambda h) = \lambda g_z(\cdot,z;h)$$

for $h,h_1,h_2\in\mathbb{C}$ and $\lambda\in\mathbb{R}$.

By linearizing the nonlinear term in the sense of

$$g(\cdot,u) - g(\cdot,u^i) \approx g_z(\cdot,u^i;u-u^i)$$

we obtain the linearized version of the forward problem

$$(\mathrm{SP_{lin}}) \quad \begin{cases} \Delta u + k^2 u = 0, & \text{in } \mathbb{R}^d \setminus \overline{D}, \\ \dfrac{\partial u}{\partial \nu} + \mathrm{i}k\Big(\lambda u - \operatorname{Div}(\mu \nabla_\tau u)\Big) - g_z(\cdot,u^i;u-u^i) = g(\cdot,u^i), & \text{on } \partial D, \\ u^s \text{ satisfies SRC}, \end{cases}$$

where the boundary condititon is $\mathbb{R}$-linear with respect to u^s. The linearization of the boundary condition provides the advantage that we can find an equivalent representation of the scattering problem ($\mathrm{SP_{lin}}$) as a boundary integral equation.

2.4.1. Boundary Integral Equation

Let $D \subseteq \mathbb{R}^d$ ($d = 2,3$) be a bounded domain with Hölder-continuous boundary $\partial D \in C^{1,1}$. This regularity assumption ensures sufficient smoothness for the analysis and boundedness of the relevant boundary integral operators involved in the subsequent study, see Lemma 2.13 below. Moreover, we assume that $\lambda \in C^1(\partial D)$ and $\mu \in C^2(\partial D)$. Using a suitable ansatz for the scattered wave, we can find an equivalent representation of the given boundary value problem as an integral equation.

In the direct approach, any solution of the Helmholtz equation in the exterior domain that satisfies the Sommerfeld radiation condition is given by the representation formula

$$u(x) = \int_{\partial D} u(y) \frac{\partial \Phi(x,y)}{\partial \nu_y} - \frac{\partial u(y)}{\partial \nu} \Phi(x,y) \, \mathrm{d}s_y \quad \text{for } x \in \mathbb{R}^d \setminus \overline{D}, \tag{2.23}$$

where Φ denotes the fundamental solution of the Helmholtz equation, which is given by

$$\Phi(x,y) = \begin{cases} \dfrac{\mathrm{i}}{4} H_0^{(1)}(k|x-y|), & d = 2, \\ \dfrac{\mathrm{e}^{\mathrm{i}k|x-y|}}{4\pi |x-y|}, & d = 3, \end{cases}$$

for $x, y \in \mathbb{R}^d$, $x \neq y$. Here, $H_0^{(1)}$ denotes the Hankel function of the first kind of order zero. In the representation formula (2.23), we have used the single-layer potential and the double-layer potential, which are both solutions to the Helmholtz equation.

Definition 2.11. Let $D \subseteq \mathbb{R}^d$ be a simply connected, bounded domain, ν the unit normal vector to ∂D and $\varphi \in C(\partial D)$. Then

$$\begin{aligned} \mathrm{SL}\varphi(x) &= \int_{\partial D} \Phi(x,y)\varphi(y) \, \mathrm{d}s_y, \quad x \in \mathbb{R}^d \setminus \partial D, \\ \mathrm{DL}\varphi(x) &= \int_{\partial D} \frac{\partial \Phi(x,y)}{\partial \nu(y)} \varphi(y) \, \mathrm{d}s_y, \quad x \in \mathbb{R}^d \setminus \partial D, \end{aligned}$$

are called single-layer and double-layer potentials with density φ on ∂D.

The single-layer and double-layer potentials fulfill the Helmholtz equation as well as the Sommerfeld radiation condition. In order to include the boundary condition, we must extend the potentials to the boundary by applying the Dirichlet trace (2.2) and the Neumann trace (2.3). The following limits can be found, for example, in [CK13, Thm. 3.1].

Using Lebesgue's dominated convergence theorem, it can be shown that the following limit exists

$$\mathrm{SL}\varphi(x)|_{\pm} = \lim_{y\to x^{\pm}} \mathrm{SL}\varphi(y) = \int_{\partial D} \Phi(x,y)\varphi(y)\,\mathrm{d}s_y, \quad x \in \partial D. \tag{2.24}$$

Here, the $(-)$ sign indicates the inner and the $(+)$ sign the outer limits of the potential on the boundary, i.e.,

$$v(x)|_+ = \lim_{y\to x^+} v(y) = \lim_{\substack{y\to x \\ y\in\mathbb{R}^d\setminus\overline{D}}} v(y) \quad \text{and} \quad v(x)|_- = \lim_{y\to x^-} v(y) = \lim_{\substack{y\to x \\ y\in D}} v(y).$$

The normal derivative of $\mathrm{SL}\varphi$ on ∂D exists in the sense that

$$\left.\frac{\partial \mathrm{SL}\varphi(x)}{\partial \nu}\right|_{\pm} = \lim_{\substack{\epsilon\to 0 \\ \epsilon>0}} [\nu(x)\cdot\nabla\mathrm{SL}\varphi(x\pm\epsilon\nu(x))]$$

converges uniformly with respect to $x \in \partial D$ and it holds that

$$\left.\frac{\partial \mathrm{SL}\varphi(x)}{\partial \nu}\right|_{\pm} = \mp\frac{1}{2}\varphi(x) + \int_{\partial D} \frac{\partial\Phi(x,y)}{\partial\nu(x)}\varphi(y)\,\mathrm{d}s_y, \quad x \in \partial D. \tag{2.25}$$

For the double-layer potential, we obtain the jump relations

$$\mathrm{DL}\varphi(x)|_{\pm} = \pm\frac{1}{2}\varphi(x) + \int_{\partial D} \frac{\partial\Phi(x,y)}{\partial\nu(y)}\varphi(y)\,\mathrm{d}s_y, \quad x \in \partial D, \tag{2.26}$$

$$\lim_{\substack{\epsilon\to 0 \\ \epsilon>0}} [\nu(x)\cdot\nabla\mathrm{DL}\varphi(x+\epsilon\nu(x)) - \nu(x)\cdot\nabla\mathrm{DL}\varphi(x-\epsilon\nu(x))] = 0. \tag{2.27}$$

From these boundary limits, we can see that the single-layer potential is continuous at the surface, but that its gradient in the normal direction is discontinuous, with a jump discontinuity equal to the density. In contrast, the double-layer potential is discontinuous at the surface, exhibiting a jump of φ, and the outer and inner Neumann traces coincide at the boundary. For the integral expressions on the right-hand side of (2.23), we introduce the following operators, see [CK13, (3.8)–(3.10)]

Definition 2.12. Let $D \subseteq \mathbb{R}^d$ be a simply connected, bounded domain, ν the unit normal vector to ∂D and $\varphi \in C(\partial D)$. On the boundary ∂D we define the single-layer and double-layer operators by

$$\mathcal{S}\varphi(x) = \int_{\partial D} \Phi(x,y)\varphi(y)\,\mathrm{d}s_y, \quad x \in \partial D,$$

$$\mathcal{D}\varphi(x) = \int_{\partial D} \frac{\partial\Phi(x,y)}{\partial\nu(y)}\varphi(y)\,\mathrm{d}s_y, \quad x \in \partial D,$$

and the adjoint double-layer operator by

$$\mathcal{D}'\varphi(x) = \int_{\partial D} \frac{\partial \Phi(x,y)}{\partial \nu(x)} \varphi(y)\,\mathrm{d}s_y, \quad x \in \partial D.$$

As an ansatz to represent the scattered wave explicitly, we use the single-layer potential

$$u^s(x) = \int_{\partial D} \Phi(x,y)\varphi(y)\,\mathrm{d}s_y, \quad x \in \mathbb{R}^d \backslash \overline{D}.$$

On the boundary ∂D, the scattered wave u^s fulfills the $\mathbb{R}$-linear generalized impedance boundary condition, which is given by

$$\frac{\partial u^s}{\partial \nu}\bigg|_+ + \mathrm{i}k\Big(\lambda - \mathrm{Div}\mu\nabla_\tau\Big)\, u^s|_+ - g_z(\cdot, u^i; u^s|_+) = -\frac{\partial u^i}{\partial \nu} - \mathrm{i}k\Big(\lambda u^i - \mathrm{Div}(\mu\nabla_\tau u^i)\Big) + g(\cdot, u^i).$$

To ensure that the boundary integral equation is well-posed, the function g_z is required to satisfy a Carathéodory condition, analogous to the one imposed on g in (2.14). Specifically, we assume

$$|g_z(x,z;w)| \le (|\psi(x)| + c|z|^p)\,|w|, \tag{2.28}$$

for almost every $x \in \partial D$ and all $z, w \in \mathbb{C}$, where $\psi \in L^2(\partial D)$, $c > 0$ and $1 \le p < \infty$. Inserting the jump conditions (2.24) and (2.25) leads to the boundary integral equation

$$-\frac{1}{2}\varphi + \mathcal{D}'\varphi + \mathrm{i}k\Big(\lambda\mathcal{S}\varphi - \mathrm{Div}(\mu\nabla_\tau\mathcal{S}\varphi)\Big) - g_z(\cdot, u^i; \mathcal{S}\varphi) = f \tag{2.29}$$

with

$$f = -\frac{\partial u^i}{\partial \nu} - \mathrm{i}k\Big(\lambda u^i - \mathrm{Div}(\mu\nabla_\tau u^i)\Big) + g(\cdot, u^i). \tag{2.30}$$

Considering this integral equation in $C(\partial D)$, the weakly singular boundary integral operators $\mathcal{S}, \mathcal{D}' \colon C(\partial D) \to C(\partial D)$ are known to be compact, see [CK13, p. 51].

By choosing the density $\varphi \in H^{\frac{1}{2}}(\partial D)$, we ensure that the solution $u = u^i + u^s$ lies in $H^2_{\mathrm{loc}}(\mathbb{R}^d \backslash \overline{D})$. In order to guarantee that the single-layer and adjoint double-layer potentials are well-defined and map continuously between the appropriate Sobolev spaces, we assume that the boundary ∂D is at least of class $C^{1,1}$.

Lemma 2.13. *Let ∂D be of class $C^{1,1}$. Then*

$$\mathcal{S} \colon H^{\frac{1}{2}}(\partial D) \to H^{\frac{3}{2}}(\partial D) \quad \text{and} \quad \mathcal{D}' \colon H^{\frac{1}{2}}(\partial D) \to H^{\frac{1}{2}}(\partial D)$$

are bounded linear operators.

Proof. See [McL00, Thm. 7.2]. □

We define the left-hand side of the integral equation (2.29) by the operator

$$A \colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D), \quad A\varphi = -\frac{1}{2}\varphi + \mathcal{D}'\varphi + \mathrm{i}k\Big(\lambda\mathcal{S}\varphi - \mathrm{Div}(\mu\nabla_\tau\mathcal{S}\varphi)\Big) - g_z(\cdot, u^i; \mathcal{S}\varphi),$$

which is bounded according to Lemma 2.13.

The integral equation (2.29) provides an equivalent formulation of the scattering problem ($\mathrm{SP}_{\mathrm{lin}}$), i.e., $u^s(x) = \mathrm{SL}\varphi$ solves the scattering problem if and only if $\varphi \in H^{\frac{1}{2}}(\partial D)$ fulfills $A\varphi = f$.

The idea for an existence result concerning the scattering problem with an $\mathbb{R}$-linear boundary condition is to use Riesz's theory analogous to the linear case. However, since we only have an $\mathbb{R}$-linear rather than a $\mathbb{C}$-linear operator, we formulate the integral equation as a system of equations in $\mathbb{R}^2$.

2.4.2. Real-linear Matrix Analysis

If $\mathbb{C}^n$ is considered to be a vector space over $\mathbb{R}$, a real-linear operator acting on $\mathbb{C}^n$ can be represented by a $2n \times 2n$ matrix. On a theoretical level, this approach is helpful for applying results from linear operator theory to $\mathbb{R}$-linear problems. However, with regard to numerical methods, it may be more advantageous to rewrite the real matrix problem in a suitable complex form, since this can prevent the convergence rate of the iterations from becoming inappropriately slow, see [Fre92]. For more detailed explanations and further matrix representations of $\mathbb{R}$-linear operators, we refer to [HN07, Ruo13, EHvP03].

Using the conjugation operator τ given by $\tau x = \overline{x}$, an $\mathbb{R}$-linear operator $\mathcal{M}$ acting on $\mathbb{C}^n$ can be written as

$$\mathcal{M} = M + M_{\#}\tau,$$

where $M, M_{\#} \in \mathbb{C}^{n\times n}$ are a pair of matrices called the complex-linear and antilinear parts of $\mathcal{M}$. In particular, M and $M_{\#}$ are represented by

$$M = \frac{1}{2}(\mathcal{M} - \mathrm{i}\mathcal{M}\mathrm{i}) \quad \text{and} \quad M_{\#} = \frac{1}{2}(\mathcal{M} + \mathrm{i}\mathcal{M}\mathrm{i})\tau\,.$$

In order to split a vector $x \in \mathbb{C}^n$ into its real and imaginary parts, we introduce the real-linear map $\mathcal{T}$ given by

$$\mathcal{T} \colon \mathbb{C}^n \to \mathbb{R}^{2n},\ x \mapsto Tx + T_{\#}\tau x = \begin{bmatrix} \mathrm{Re}(x) \\ \mathrm{Im}(x) \end{bmatrix},$$

where T is the complex-linear and $T_{\#}$ the antilinear part of $\mathcal{T}$. These matrices are defined as

$$T = \frac{1}{2}\begin{bmatrix} I \\ -\mathrm{i}I \end{bmatrix} \quad \text{and} \quad T_{\#} = \overline{T} = \frac{1}{2}\begin{bmatrix} I \\ \mathrm{i}I \end{bmatrix}.$$

We equip $\mathbb{C}^n$ with the real-valued inner product $\langle x, y\rangle_{\mathbb{C}^n} = \mathrm{Re}(x^*y)$, and $\mathbb{R}^{2n}$ with the standard Euclidean inner product. With respect to these inner products, $\mathcal{T}$ is an isometry and satisfies $\mathcal{T}^* = \mathcal{T}^{-1}$.

A common method for dealing with $\mathbb{R}$-linear problems is to use a real matrix representation $\phi(\mathcal{M})$ of the operator, while the vector spaces are considered to be over $\mathbb{R}$. A real matrix representation of $\mathcal{M}$ is given by

$$\phi(\mathcal{M}) = \begin{bmatrix} \mathrm{Re}(M + M_{\#}) & -\mathrm{Im}(M - M_{\#}) \\ \mathrm{Im}(M + M_{\#}) & \mathrm{Re}(M - M_{\#}) \end{bmatrix},$$

which yields the identity

$$\mathcal{T}\mathcal{M} = \phi(\mathcal{M})\mathcal{T}, \quad \text{i.e.,} \quad \mathcal{M} = \mathcal{T}^* \phi(\mathcal{M})\mathcal{T}\,.$$

Remark 2.14. The mapping ϕ is bijective, isometric, and

$$\phi(\mathcal{M}_1 + \mathcal{M}_2) = \phi(\mathcal{M}_1) + \phi(\mathcal{M}_2), \quad \phi(\mathcal{M}_1\mathcal{M}_2) = \phi(\mathcal{M}_1)\phi(\mathcal{M}_2)$$

for $\mathbb{R}$-linear operators $\mathcal{M}_1$ and $\mathcal{M}_2$ of the same size, see [HN07, Sec. 5.1]. ♢

We now consider the corresponding integral equation formulation $A\varphi = f$ of the $\mathbb{R}$-linear scattering problem ($\mathrm{SP}_{\mathrm{lin}}$), where the operator A is given by

$$A\varphi = -\frac{1}{2}\varphi + \mathcal{D}'\varphi + \mathrm{i}k\Big(\lambda\mathcal{S}\varphi - \mathrm{Div}(\mu\nabla_\tau\mathcal{S}\varphi)\Big) - g_z(\cdot, u^i; \mathcal{S}\varphi), \quad \varphi \in H^{\frac{1}{2}}(\partial D),$$

and the right-hand side f is defined as in (2.30). Due to the fact that only the function g_z is $\mathbb{R}$-linear and the remaining part of the operator is $\mathbb{C}$-linear, we first decompose A into

$$A = A_{\mathbb{C}-\mathrm{lin}} + A_{\mathbb{R}-\mathrm{lin}}\,,$$

where $A_{\mathbb{R}-\mathrm{lin}}\varphi = -g_z(\cdot, u^i; \mathcal{S}\varphi)$. Next, we split the $\mathbb{R}$-linear operator into its complex-linear and antilinear part, i.e.,

$$A_{\mathbb{R}-\mathrm{lin}} = G + G_\# \tau\,.$$

In our case, applying the operators G and $G_\#$ to $\varphi \in H^{\frac{1}{2}}(\partial D)$ results in

$$G\varphi = \frac{1}{2}A_{\mathbb{R}-\mathrm{lin}}\varphi - \frac{\mathrm{i}}{2}A_{\mathbb{R}-\mathrm{lin}}(\mathrm{i}\varphi) = -\frac{1}{2}\Big(g_z(\cdot, u^i; \mathcal{S}\varphi) - \mathrm{i}g_z(\cdot, u^i; \mathcal{S}\mathrm{i}\varphi)\Big)\,, \tag{2.31}$$

$$G_\#\varphi = \frac{1}{2}A_{\mathbb{R}-\mathrm{lin}}(\tau\varphi) + \frac{\mathrm{i}}{2}A_{\mathbb{R}-\mathrm{lin}}(\mathrm{i}\tau\varphi) = -\frac{1}{2}\Big(g_z(\cdot, u^i; \mathcal{S}\overline{\varphi}) + \mathrm{i}g_z(\cdot, u^i; \mathcal{S}\mathrm{i}\overline{\varphi})\Big)\,. \tag{2.32}$$

Therefore, the real matrix representation of A is given by

$$\begin{aligned}
\phi(A) &= \phi(A_{\mathbb{C}-\mathrm{lin}} + A_{\mathbb{R}-\mathrm{lin}}) = \phi(A_{\mathbb{C}-\mathrm{lin}}) + \phi(A_{\mathbb{R}-\mathrm{lin}}) \\
&= \begin{pmatrix} \mathrm{Re}(A_{\mathbb{C}-\mathrm{lin}}) & -\mathrm{Im}(A_{\mathbb{C}-\mathrm{lin}}) \\ \mathrm{Im}(A_{\mathbb{C}-\mathrm{lin}}) & \mathrm{Re}(A_{\mathbb{C}-\mathrm{lin}}) \end{pmatrix} + \begin{pmatrix} \mathrm{Re}(G + G_\#) & -\mathrm{Im}(G - G_\#) \\ \mathrm{Im}(G + G_\#) & \mathrm{Re}(G - G_\#) \end{pmatrix} \\
&= \begin{pmatrix} \mathrm{Re}(A_{\mathbb{C}-\mathrm{lin}} + G + G_\#) & -\mathrm{Im}(A_{\mathbb{C}-\mathrm{lin}} + G - G_\#) \\ \mathrm{Im}(A_{\mathbb{C}-\mathrm{lin}} + G + G_\#) & \mathrm{Re}(A_{\mathbb{C}-\mathrm{lin}} + G - G_\#) \end{pmatrix}\,.
\end{aligned} \tag{2.33}$$

With (2.31) and (2.32), we see that the operators under consideration are defined by

$$\begin{aligned}
(A_{\mathbb{C}-\mathrm{lin}} + G + G_\#)\varphi = -\frac{1}{2}\varphi + \mathcal{D}'\varphi + \mathrm{i}k\Big(\lambda\mathcal{S}\varphi - \mathrm{Div}(\mu\nabla_\tau\mathcal{S}\varphi)\Big) - \frac{1}{2}g_z(\cdot, u^i; \mathcal{S}(\varphi + \overline{\varphi})) \\
+ \frac{\mathrm{i}}{2}g_z(\cdot, u^i; \mathcal{S}\mathrm{i}(\varphi - \overline{\varphi})),
\end{aligned}$$

$$
\begin{aligned}
(A_{\mathbb{C}-\mathrm{lin}} + G - G_{\#})\varphi = -\frac{1}{2}\varphi + \mathcal{D}'\varphi + \mathrm{i}k\Big(\lambda\mathcal{S}\varphi - \mathrm{Div}(\mu\nabla_\tau\mathcal{S}\varphi)\Big) - \frac{1}{2}g_z(\cdot, u^i; \mathcal{S}(\varphi - \overline{\varphi}))\\
+ \frac{\mathrm{i}}{2}g_z(\cdot, u^i; \mathcal{S}\mathrm{i}(\varphi + \overline{\varphi})),
\end{aligned}
$$

for $\varphi \in H^{\frac{1}{2}}(\partial D)$. Thus, a real representation of the integral equation $A\varphi = f$ is provided by

$$
\phi(A)\begin{pmatrix}\mathrm{Re}\,(\varphi)\\ \mathrm{Im}\,(\varphi)\end{pmatrix} = \begin{pmatrix}\mathrm{Re}\,(f)\\ \mathrm{Im}\,(f)\end{pmatrix}. \tag{2.34}
$$

The aim now is to show the well-posedness of the $\mathbb{R}$-linear problem ($\mathrm{SP}_{\mathrm{lin}}$) using linear existence and uniqueness theory.

2.4.3. Well-posedness in H^2_{loc}

As in Section 2.3.1, we apply Rellich's lemma to establish the following uniqueness result.

Theorem 2.15. *Let* $\mathrm{Re}(\mu) \geq 0$ *and*

$$
k\mathrm{Re}(\lambda) \geq \sup_{z,w\in\mathbb{C}} \frac{\mathrm{Im}(g_z(x,z;w)\overline{w})}{|w|^2} \quad \textit{for any } z, w \in \mathbb{C} \textit{ and a.e. } x \in \partial D.
$$

Then, any solution $u \in H^2_{\mathrm{loc}}(\mathbb{R}^d\backslash\overline{D})$ *to the homogeneous problem* (SP_{lin}) *vanishes identically. Consequently, the* $\mathbb{R}$*-linear scattering problem has at most one solution.*

Proof. Analogous to the proof of Theorem 2.6. □

In order to obtain an existence result for the scattering problem with an $\mathbb{R}$-linear boundary condition, we use the existence theory based on Riesz theory analogously to the linear case. The following theorem is a corollary of Riesz's third theorem and states that injective compact perturbations of the identity are boundedly invertible, see [Kre14, Thm. 3.4].

Theorem 2.16. *Let* X *be a normed space,* $K\colon X \to X$ *a compact operator, and* $I - K\colon X \to X$ *injective. Then* $I - K$ *is bijective with bounded inverse* $(I-K)^{-1} \in \mathcal{L}(X, X)$.

The aim is now to apply this theorem to the integral equation system (2.34). This procedure is based on the existence proof in [Kre19], whereby we must also take the function g_z into account. Initially, we need a real matrix representation of the operator A having the form

$$
\phi(A) = \phi(B)\left[\begin{pmatrix} I & 0\\ 0 & I\end{pmatrix} - \begin{pmatrix}\mathrm{Re}(K+K_{\#}) & -\mathrm{Im}(K-K_{\#})\\ \mathrm{Im}(K+K_{\#}) & \mathrm{Re}(K-K_{\#})\end{pmatrix}\right],
$$

where B is a boundedly invertible operator and $K + K_{\#}$, $K - K_{\#}$ are compact operators. Therefore, we introduce the operator

$$
L\colon H^{\frac{3}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D), \quad L\varphi = -\mathrm{Div}\nabla_\tau\varphi + \varphi,
$$

which is also known as the modified Laplace-Beltrami operator, see [Kre19]. Here, the notation Δ_τ can also be used instead of $\mathrm{Div}\nabla_\tau$. If the operator $\mathrm{i}k\mu L\mathcal{S}\colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D)$ is boundedly invertible, $\phi(A)$ has the representation

$$\begin{aligned}\phi(A) &= \phi(\mathrm{i}k\mu LS + A - \mathrm{i}k\mu LS) = \phi\left((\mathrm{i}k\mu LS)(I + (\mathrm{i}k\mu LS)^{-1}(A - \mathrm{i}k\mu LS)\right) \\ &= \phi(\mathrm{i}k\mu LS)\left[\phi(I) + \phi((\mathrm{i}k\mu LS)^{-1})\phi(A - \mathrm{i}k\mu LS)\right].\end{aligned}$$

For a more concise formulation, we use the notation $B := \mathrm{i}k\mu LS$. Using the real matrix representation (2.33) of A, this thus yields

$$\phi(A) = \phi(B)\left[\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} + \phi(B^{-1})\begin{pmatrix} \mathrm{Re}(A_{\mathbb{C}-\mathrm{lin}} - B + G + G_{\#}) & -\mathrm{Im}(A_{\mathbb{C}-\mathrm{lin}} - B + G - G_{\#}) \\ \mathrm{Im}(A_{\mathbb{C}-\mathrm{lin}} - B + G + G_{\#}) & \mathrm{Re}(A_{\mathbb{C}-\mathrm{lin}} - B + G - G_{\#}) \end{pmatrix}\right].$$

According to this, we obtain the unique solvability of the system (2.34) with Theorem 2.16, by showing the following statements

- $\mathrm{i}k\mu L\mathcal{S}\colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D)$ is an isomorphism,
- $A_{\mathbb{C}-\mathrm{lin}} - \mathrm{i}k\mu LS + G + G_{\#}\colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D)$ and $A_{\mathbb{C}-\mathrm{lin}} - \mathrm{i}k\mu LS + G - G_{\#}\colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D)$ are compact,
- $A\colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D)$ is injective.

Using Riesz theory, the existence of a solution $u \in H^2_{\mathrm{loc}}(\mathbb{R}^d \setminus \overline{D})$ to the scattering problem ($\mathrm{SP}_{\mathrm{lin}}$) can be concluded from the uniqueness of a solution to the integral equation.

For the integral equation formulation, we choose a single-layer potential ansatz, which, however, requires a restriction to the wave number k in order to prove uniqueness. If k^2 is a Dirichlet eigenvalue of the negative Laplacian in D, the injectivity of the single-layer operator $\mathcal{S}$ is no longer given, and thus $\mathcal{S}\colon H^{\frac{1}{2}}(\partial D) \to H^{\frac{3}{2}}(\partial D)$ is not an isomorphism in this case, see [CC14, Thm. 7.3].

Lemma 2.17. *Let $\lambda \in C^1(\partial D)$, $\mu \in C^2(\partial D)$ with $|\mu| > 0$ and k^2 not a Dirichlet eigenvalue of $-\Delta$ in D. Then the operator*

$$\mathrm{i}k\mu L\mathcal{S}\colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D), \quad \varphi \mapsto \mathrm{i}k\mu(-\mathrm{Div}\nabla_\tau \mathcal{S}\varphi + \mathcal{S}\varphi)$$

is an isomorphism.

Proof. The boundedness of the single-layer operator $\mathcal{S}\colon H^{\frac{1}{2}}(\partial D) \to H^{\frac{3}{2}}(\partial D)$ is provided by Lemma 2.13. Since k^2 is not a Dirichlet eigenvalue of $-\Delta$ in D by assumption, it follows that $\mathcal{S}\colon H^{\frac{1}{2}}(\partial D) \to H^{\frac{3}{2}}(\partial D)$ is an isomorphism. In order to show that L is also an isomorphism, the Sobolev interpolation argument from [McL00, Thm. B.11] can be used, i.e., it suffices to show that the operators

$$\begin{aligned} L_1&\colon H^1(\partial D) \to H^{-1}(\partial D), && \varphi \mapsto -\mathrm{Div}\nabla_\tau\varphi + \varphi, \\ L_2&\colon H^2(\partial D) \to L^2(\partial D), && \varphi \mapsto -\mathrm{Div}\nabla_\tau\varphi + \varphi \end{aligned}$$

are isomorphisms. For the proof of these two statements, we refer to [Kre19, Lemma 2.4]. If we now assume $|\mu| > 0$, we can finally conclude that the operator $\mathrm{i}k\mu L\mathcal{S}\colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D)$ is an isomorphism. □

Next, we show the compactness of the operators $A_{\mathbb{C}-\text{lin}}-\text{i}k\mu LS+G\pm G_{\#}\colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D)$. To ensure the boundedness of the operators on $H^{\frac{1}{2}}(\partial D)$, we rely on the growth condition for the function g_z as defined in (2.28).

Lemma 2.18. *Let $\lambda \in C^1(\partial D)$, $\mu \in C^2(\partial D)$ with $|\mu| > 0$ and k^2 not a Dirichlet eigenvalue of $-\Delta$ in D. Moreover, the linearization g_z fulfills the growth condition* (2.28)*. Then the operators*

$$A_{\mathbb{C}-\text{lin}} - \text{i}k\mu LS + G + G_{\#}\colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D),$$
$$A_{\mathbb{C}-\text{lin}} - \text{i}k\mu LS + G - G_{\#}\colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D)$$

are compact.

Proof. Under the given assumptions on λ, μ and k the operators $A_{\mathbb{C}-\text{lin}}\colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D)$ and $\text{i}k\mu L\mathcal{S}\colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D)$ are bounded.

Applying the product rule to the surface divergence term yields

$$\text{Div}\mu\nabla_\tau\mathcal{S}\varphi = \mu\text{Div}\nabla_\tau\mathcal{S}\varphi + \nabla_\tau\mu \cdot \nabla_\tau\mathcal{S}\varphi.$$

Subtracting both operators leads to

$$\begin{aligned}(A_{\mathbb{C}-\text{lin}} - \text{i}k\mu L\mathcal{S})\varphi &= -\frac{1}{2}\varphi + \mathcal{D}'\varphi + \text{i}k\Big(\lambda\mathcal{S}\varphi - \text{Div}(\mu\nabla_\tau\mathcal{S}\varphi)\Big) - \text{i}k\mu\Big(-\text{Div}\nabla_\tau\mathcal{S}\varphi + \mathcal{S}\varphi\Big)\\ &= -\frac{1}{2}\varphi + \mathcal{D}'\varphi + \text{i}k\lambda\mathcal{S}\varphi - \text{i}k\nabla_\tau\mu \cdot \nabla_\tau\mathcal{S}\varphi - \text{i}k\mu\mathcal{S}\varphi\end{aligned}$$

for all $\varphi \in H^{\frac{1}{2}}(\partial D)$, see [Kre19, Lem. 2.5]. Using Lemma 2.13 yields the boundedness of the operator $A_{\mathbb{C}-\text{lin}} - \text{i}k\mu L\mathcal{S}\colon H^{\frac{1}{2}}(\partial D) \to H^{\frac{1}{2}}(\partial D)$. The compactness of the operator then follows from the compact embedding $H^{\frac{1}{2}}(\partial D) \hookrightarrow H^{-\frac{1}{2}}(\partial D)$. Furthermore, the growth condition (2.28) for g_z implies the boundedness of $G + G_{\#}\colon H^{\frac{1}{2}}(\partial D) \to L^2(\partial D)$, since

$$\begin{aligned}\|(G + G_{\#})\varphi\|_{L^2(\partial D)} &\leq \frac{1}{2}\big\|g_z(\cdot, u^i; \mathcal{S}(\varphi + \overline{\varphi}))\big\|_{L^2(\partial D)} + \frac{1}{2}\big\|g_z(\cdot, u^i; \mathcal{S}\text{i}(\varphi - \overline{\varphi}))\big\|_{L^2(\partial D)}\\ &\leq \frac{1}{2}\big\|(|\psi| + c|u^i|^p)|\mathcal{S}(\varphi + \overline{\varphi})|\big\|_{L^2(\partial D)} + \frac{1}{2}\big\|(|\psi| + c|u^i|^p)|\mathcal{S}\text{i}(\varphi - \overline{\varphi})|\big\|_{L^2(\partial D)}\\ &\leq \frac{1}{2}\left(\|\psi\|_{L^2(\partial D)} + c\|u^i\|^p_{L^2(\partial D)}\right)\|\mathcal{S}(\varphi + \overline{\varphi})\|_{L^\infty(\partial D)}\\ &\quad + \frac{1}{2}\left(\|\psi\|_{L^2(\partial D)} + c\|u^i\|^p_{L^2(\partial D)}\right)\|\mathcal{S}\text{i}(\varphi - \overline{\varphi})\|_{L^\infty(\partial D)}\\ &\leq C\left(\|\psi\|_{L^2(\partial D)} + c\|u^i\|^p_{L^2(\partial D)}\right)\|\varphi\|_{H^{\frac{1}{2}}(\partial D)},\end{aligned}$$

where Hölder's inequality is used in the third estimate, and the final step relies on the continuity of the single-layer operator $\mathcal{S}\colon H^{\frac{1}{2}}(\partial D) \to L^\infty(\partial D)$, see Theorem 2.21. To prove compactness, we consider the following composition of operators:

$$H^{\frac{1}{2}}(\partial D) \xrightarrow{\mathcal{S}} H^{\frac{3}{2}}(\partial D) \xhookrightarrow{\text{compact}} L^2(\partial D) \xrightarrow{g_z(\cdot,u^i;\cdot)} L^2(\partial D) \xhookrightarrow{\text{continuous}} H^{-\frac{1}{2}}(\partial D)\,,$$

where $g_z(\cdot, u^i; \cdot)$ denotes the Nemytskii operator induced by g_z. Since $\mathcal{S}$ and $g_z(\cdot, u^i; \cdot)$ are bounded and the embedding $H^{3/2}(\partial D) \hookrightarrow L^2(\partial D)$ is compact, the operator

$$G + G_{\#} \colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D)$$

is compact. Analogously, we obtain the compactness of the operator $G - G_{\#} \colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D)$, which ultimately leads to the statement of the lemma. □

Lemma 2.19. *Let $\lambda \in C^1(\partial D)$, $\mu \in C^2(\partial D)$ and k^2 not a Dirichlet eigenvalue of $-\Delta$ in D. Then the operator*

$$A \colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D)$$

is injective.

Proof. Let $\varphi \in H^{\frac{1}{2}}(\partial D)$ with $A\varphi = 0$ and $v = \mathrm{SL}\varphi$. Then v solves the scattering problem

$$\begin{cases} \Delta v + k^2 v = 0, & \text{in } \mathbb{R}^d \backslash \overline{D}, \\ \dfrac{\partial v}{\partial \nu} + \mathrm{i}k\Big(\lambda v - \mathrm{Div}(\mu \nabla_\tau v)\Big) - g_z(\cdot, u^i; v) = 0, & \text{on } \partial D, \\ v \text{ satisfies SRC.} \end{cases}$$

Due to the uniqueness of a solution to the linearized scattering problem as stated in Theorem 2.15, it follows that $v = 0$ in $\mathbb{R}^d \backslash \overline{D}$. If we apply the continuous Dirichlet trace

$$\gamma_0^{\mathrm{ext}} \colon H^1(\mathbb{R}^d \backslash \overline{D}) \to H^{\frac{1}{2}}(\partial D), \quad \gamma_0^{\mathrm{ext}} v = v|_{\partial D},$$

we can conclude that $\mathcal{S}\varphi = 0$. Due to the injectivity of the boundary integral operator $\mathcal{S}$, it follows that $\varphi = 0$. □

In summary, we have established the existence and uniqueness of a solution $u \in H^2_{\mathrm{loc}}(\mathbb{R}^d \backslash \overline{D})$ to the linearized scattering problem ($\mathrm{SP_{lin}}$) for any fixed $k > 0$ such that k^2 is not a Dirichlet eigenvalue of $-\Delta$ in D.

Remark 2.20. This existence result can be generalized and formulated for any choice of $k > 0$ by using a combined potential approach for the scattered wave u^s, since the single layer potential approach fails if k^2 is a Dirichlet eigenvalue of $-\Delta$ in D, see [Kre18, Kre19].

Another possibility to overcome the restriction on k, is to utilize the technique of the modified Green's function, where Φ is replaced by a different fundamental solution, see [YZZ14] and the references therein. ◊

2.5. Well-posedness via Fixed Point Theory

We have shown the well-posedness of the scattering problem (SP) in $H^1_{\mathrm{loc}}(\mathbb{R}^d \backslash \overline{D})$ using the variational formulation and of ($\mathrm{SP_{lin}}$) in $H^2_{\mathrm{loc}}(\mathbb{R}^d \backslash \overline{D})$ using the boundary integral equation method. Another possibility to prove the well-posedness of the scattering problem (SP) is the application of Banach's fixed-point theorem. Then we can demand a slightly weaker assumption on g than the sublinearity condition (2.16), but we must keep the norm of the incident field small in order to obtain a contraction mapping. For the sake of extending the previous existence and uniqueness results, we carry out the proof using Banach's fixed-point theorem. The proof is based on the work [GKM22], where a nonlinear Helmholtz equation with compactly supported inhomogeneous scattering objects described by a nonlinear refractive index was considered.

In the following, we restrict ourselves to the case $\mu = 0$. This is due to the fact that in the present L^∞-based framework, the boundary integral term $\mathcal{S}\big(\mathrm{Div}(\mu\nabla_\tau u)\big)$ is not well-defined. Considering $\mu \neq 0$ would require either a formulation in stronger Sobolev spaces or additional regularity assumptions for μ and the solution u, which we will not discuss in detail here. For the impedance function λ, we again assume $\lambda \in C^1(\partial D)$.

Green's representation theorem in the exterior domain ([CK13, Thm. 2.1]) states

$$u^s(x) = \int_{\partial D} \left(\frac{\partial \Phi(x,y)}{\partial \nu_y} u(y) - \Phi(x,y) \frac{\partial u(y)}{\partial \nu} \right) \mathrm{d}s_y = \mathrm{DL}u(x) - \mathrm{SL}\frac{\partial u(x)}{\partial \nu}, \quad x \in \mathbb{R}^d \backslash \overline{D}\,.$$

Taking the limit to the boundary ∂D in Huygens' principle (see [CK13, Thm. 3.14]) and including the boundary condition from (SP), we obtain the equation

$$\begin{aligned} u^s(x) - 2\mathcal{D}u^s(x) - 2\mathcal{S}\Big(\mathrm{i}k\lambda u^s(x) - g\big(x, u^s(x) + u^i(x)\big)\Big) \\ = u^i(x) + 2\mathcal{D}u^i(x) + 2\mathcal{S}\big(\mathrm{i}k\lambda u^i(x)\big) \end{aligned} \tag{2.35}$$

for $x \in \partial D$, where $\mathcal{S}$ and $\mathcal{D}$ are the boundary integral operators defined in Definition 2.12. For the representation to hold pointwise, we assume the following regularity of the boundary, depending on the dimension $d \in \{2,3\}$, see [Kir89, Thm. 4.2 (b), Thm. 4.3 (a)].

Theorem 2.21. *Let $\alpha \in (0,1)$.*

(i) *Let $\partial D \subseteq \mathbb{R}^2$ with $\partial D \in C^{2,\alpha}$. Then $\mathcal{S}, \mathcal{D} \colon L^2(\partial D) \to H^1(\partial D) \subseteq L^\infty(\partial D)$.*

(ii) *Let $\partial D \subseteq \mathbb{R}^3$ with $\partial D \in C^{3,\alpha}$. Then $\mathcal{S}, \mathcal{D} \colon H^1(\partial D) \to H^2(\partial D) \subseteq L^\infty(\partial D)$.*

The linear part of the operator on the left-hand side in (2.35) is the adjoint of $A_{\mathbb{C}-\mathrm{lin}}$ from Section 2.4.2 with respect to the L^2 bilinear form. Therefore, we assume throughout this section that k^2 is not a Dirichlet eigenvalue of the negative Laplacian in D.

As in [GKM22], we restrict ourselves to nonlinearities of the form

$$g(x, u(x)) = \widetilde{g}(x, |u(x)|)u(x), \quad x \in \partial D,$$

where $\widetilde{g}$ is a real-valued function. In the linear case, we set $\widetilde{g}(x, |u(x)|) = g_0(x)$.

Similarly to the previous sections, we assume that the function $g(x,z)$ is measurable on ∂D, continuous with respect to $z \in \mathbb{C}$, and fulfills the condition

$$\|\widetilde{g}(\cdot, |z_1|)z_1 - \widetilde{g}(\cdot, |z_2|)z_2 - g_0(\cdot)(z_1 - z_2)\|_{L^\infty(\partial D)} \le C_g(|z_1|^p + |z_2|^p)|z_1 - z_2| \tag{2.36}$$

for a constant $C_g > 0$ and $p > 0$, $|z_1|, |z_2| \le 1$. This condition immediately implies

$$\|\widetilde{g}(\cdot, |z|)z - g_0 z\|_{L^\infty(\partial D)} \le C_g |z|^{p+1}, \quad z \in \mathbb{C},\ |z| \le 1\,, \tag{2.37}$$

with $C_g > 0$ and $p > 0$.

We denote the solution of the corresponding linear problem by u_0^s. Then the associated boundary integral equation (2.35) is given by

$$\begin{aligned} u_0^s(x) - 2\mathcal{D}u_0^s(x) - 2\mathcal{S}\Big(\mathrm{i}k\lambda u_0^s(x) - g_0(x)u_0^s(x)\Big) & \\ = u^i(x) + 2\mathcal{D}u^i(x) + 2\mathcal{S}\Big(\mathrm{i}k\lambda u^i(x) - g_0(x)u^i(x)\Big) & \end{aligned} \tag{2.38}$$

for $x \in \partial D$. In the context of a linear scattering problem, we can prove the well-posedness using the linear Riesz-Fredholm theory, as we did in the previous Section 2.4.3. Utilizing Theorem 2.16, we establish that the operator

$$\Big(I - 2\mathcal{D} - 2\mathcal{S}(\mathrm{i}k\lambda\cdot) + 2\mathcal{S}(g_0\cdot)\Big) \colon L^\infty(\partial D) \to L^\infty(\partial D)$$

is bijective and its inverse is bounded. Consequently, there exists a constant $C > 0$ such that

$$\left\| \Big(I - 2\mathcal{D} - 2\mathcal{S}(\mathrm{i}k\lambda\cdot) + 2\mathcal{S}(g_0\cdot)\Big)^{-1} q \right\|_{L^\infty(\partial D)} \le C\|q\|_{L^\infty(\partial D)} \tag{2.39}$$

for $q \in L^\infty(\partial D)$. Furthermore, the unique solution $u_0^s \in L^\infty(\partial D)$ of (2.38) is given by

$$u_0^s = \Big(I - 2\mathcal{D} - 2\mathcal{S}(\mathrm{i}k\lambda\cdot) + 2\mathcal{S}(g_0\cdot)\Big)^{-1} \Big(u^i + 2\mathcal{D}u^i + 2\mathcal{S}\left(\mathrm{i}k\lambda u^i - g_0 u^i\right)\Big).$$

Next, we introduce the linear operator $V_0 \colon L^\infty(\partial D) \to L^\infty(\partial D)$, which maps the incident field u^i onto the scattered field u_0^s, which is a solution of the linear problem (2.38), i.e., $V_0 u^i = u_0^s$. Analogously, we define the nonlinear operator $V \colon L^\infty(\partial D) \to L^\infty(\partial D)$ by $V(u^i) = u^s$, where u^s is the solution of the nonlinear scattering problem (2.35). In addition, the linear theory yields the estimate

$$\|V_0 u^i\|_{L^\infty(\partial D)} \le c\|u^i\|_{L^\infty(\partial D)}\,. \tag{2.40}$$

The aim is now to show the well-posedness of the nonlinear scattering problem using Banach's fixed point theorem. To achieve this, we consider the neighborhood

$$\mathcal{U}_\delta := \Big\{u \in L^\infty(\partial D) \mid \|u\|_{L^\infty(\partial D)} \le \delta\Big\} \quad \text{for} \quad \delta > 0.$$

Theorem 2.22. *Assume that the function $g \colon \partial D \times \mathbb{C} \to \mathbb{C}$ satisfies condition* (2.36) *or, respectively,* (2.37)*. Then there exists a $\delta > 0$ such that for any given $u^i \in \mathcal{U}_\delta$ the nonlinear integral equation* (2.35) *has a unique solution $u = V(u^i) + u^i \in L^\infty(\partial D)$ satisfying $u^s - V_0 u^i \in \mathcal{U}_\delta$. Furthermore, there exists a constant $C > 0$ such that*

$$\begin{aligned} \|V(u^i)\|_{L^\infty(\partial D)} &\le C\|u^i\|_{L^\infty(\partial D)}\,, \\ \|V(u^i) - V_0 u^i\|_{L^\infty(\partial D)} &\le C\|u^i\|^{1+p}_{L^\infty(\partial D)}\,. \end{aligned}$$

Proof. We define the nonlinear map $M \colon L^\infty(\partial D) \to L^\infty(\partial D)$ by

$$M(v) = \Big(I - 2\mathcal{D} - 2\mathcal{S}(\mathrm{i}k\lambda\cdot) + 2\mathcal{S}(g_0\cdot)\Big)^{-1} \Big(-2\mathcal{S}\widetilde{g}_{\mathrm{nl}}(\cdot, |v + u_0^s + u^i|)(v + u_0^s + u^i)\Big)\,,$$

where $\widetilde{g}_{nl} = \widetilde{g} - g_0$ contains only the nonlinear part of $\widetilde{g}$. If we can show that

$$\|M(v)\|_{L^\infty(\partial D)} \leq \delta \quad \text{and} \quad \|M(v_1) - M(v_2)\|_{L^\infty(\partial D)} \leq \frac{1}{2}\|v_1 - v_2\|_{L^\infty(\partial D)},$$

then $M\colon \mathcal{U}_\delta \to \mathcal{U}_\delta$ is a contraction, and Banach's fixed point theorem yields the existence of a uniquely determined fixed point $v \in \mathcal{U}_\delta$ of M.

Using (2.37), (2.39) and (2.40) we obtain

$$\begin{aligned}
\|M(v)\|_{L^\infty(\partial D)} &\leq C\|2\mathcal{S}\widetilde{g}_{\mathrm{nl}}(\cdot, |v + u_0^s + u^i|)(v + u_0^s + u^i)\|_{L^\infty(\partial D)} \\
&\leq C\Big(2\|\mathcal{S}\|C_g\|v + u_0^s + u^i\|_{L^\infty(\partial D)}^{1+p}\Big) \\
&\leq C\Big(2\|\mathcal{S}\|C_g(\delta + c\delta + \delta)^{1+p}\Big) = C\Big(2\|S\|C_g((2+c)\delta)^{1+p}\Big) \\
&\leq C\Big(2\|\mathcal{S}\|(2+c)C_g\delta\Big)\,,
\end{aligned}$$

assuming that $\delta \leq 1/(2+c)$ to ensure the last estimate. Choosing $\delta > 0$ such that $C_g\delta > 0$ is sufficiently small, we find that $\|M(v)\|_{L^\infty(\partial D)} \leq \delta$.

To show the second inequality, we use (2.40) and assumption (2.36). For $v_1, v_2 \in \mathcal{U}_\delta$, we then obtain

$$\begin{aligned}
&\|M(v_1) - M(v_2)\|_{L^\infty(\partial D)} \\
&\qquad \leq C\|\mathcal{S}\|\|\widetilde{g}_{\mathrm{nl}}(\cdot, |v_1 + u_0^s + u^i|)(v_1 + u_0^s + u^i) - \widetilde{g}_{\mathrm{nl}}(\cdot, |v_2 + u_0^s + u^i|)(v_2 + u_0^s + u^i)\|_{L^\infty(\partial D)} \\
&\qquad \leq C\|\mathcal{S}\|C_g\Big(\|v_1 + u_0^s + u^i\|_{L^\infty(\partial D)}^p + \|v_2 + u_0^s + u^i\|_{L^\infty(\partial D)}^p\Big)\|v_1 - v_2\|_{L^\infty(\partial D)} \\
&\qquad \leq C\|\mathcal{S}\|C_g 2(\delta + c\delta + \delta)^p\|v_1 - v_2\|_{L^\infty(\partial D)} \\
&\qquad \leq C\|\mathcal{S}\|2(2+c)C_g\delta\|v_1 - v_2\|_{L^\infty(\partial D)}\,,
\end{aligned}$$

where the last estimate again follows from $\delta \leq 1/(2+c)$. Choosing $\delta > 0$ such that $C_g\delta > 0$ is sufficiently small, we find that

$$\|M(v_1) - M(v_2)\|_{L^\infty(\partial D)} \leq \frac{1}{2}\|v_1 - v_2\|_{L^\infty(\partial D)}\,.$$

So with a sufficiently small incident field, Banach's fixed point theorem provides a uniquely determined fixed point $v \in \mathcal{U}_\delta$ of M.

Now it is still left to establish the connection between the mapping M and the solution to the integral equation (2.35). The scattered field $u^s \in L^\infty(\partial D)$ solves the integral equation (2.35) if and only if $v = u^s - u_0^s$ satisfies

$$v - 2\mathcal{D}v - 2\mathcal{S}\left(\mathrm{i}k\lambda v - g_0 v\right) = -2\mathcal{S}\left(g(\cdot, u^s + u^i) - g_0 u_0^s\right) = -2\mathcal{S}\widetilde{g}_{\mathrm{nl}}(\cdot, |v + u_0^s + u^i|)(v + u_0^s + u^i)\,,$$

which is equivalent to the fixed-point equation $v = M(v)$.

The estimate of the norm of $V(u^i) - V_0 u^i$ follows from (2.37) and (2.39), because

$$
\begin{aligned}
&\|V(u^i) - V_0 u^i\|_{L^\infty(\partial D)} = \left\| M\left(V(u^i) - V_0 u^i\right)\right\|_{L^\infty(\partial D)} \\
&= \left\| \Big(I - 2\mathcal{D} - 2\mathrm{i}k\mathcal{S}(\lambda\cdot) - 2\mathcal{S}(g_0\cdot)\Big)^{-1} \ \Big(-2\mathcal{S}\widetilde{g}_{\mathrm{nl}}(\cdot, |V(u^i) + u^i|)(V(u^i) + u^i)\Big)\right\|_{L^\infty(\partial D)} \\
&\leq C\|\mathcal{S}\| \|\widetilde{g}_{\mathrm{nl}}(\cdot, |V(u^i) + u^i|)(V(u^i) + u^i)\|_{L^\infty(\partial D)} \\
&\leq C\|\mathcal{S}\| C_g \|V(u^i) + u^i\|^{1+p}_{L^\infty(\partial D)} \\
&\leq C\|\mathcal{S}\| C_g \Big(\|V(u^i) - V_0 u^i\|_{L^\infty(\partial D)} + \|V_0 u^i + u^i\|_{L^\infty(\partial D)}\Big)^p \|V(u^i) + u^i\|_{L^\infty(\partial D)} \,.
\end{aligned} \tag{2.41}
$$

Using (2.40) and (2.41) yields

$$
\begin{aligned}
&\|V(u^i)\|_{L^\infty(\partial D)} = \|V_0 u^i + V(u^i) - V_0 u^i\|_{L^\infty(\partial D)} \\
&\leq C\|u^i\|_{L^\infty(\partial D)} + \|V(u^i) - V_0 u^i\|_{L^\infty(\partial D)} \\
&\leq C\|u^i\|_{L^\infty(\partial D)} + C\|\mathcal{S}\| C_g \Big(\|V(u^i) - V_0 u^i\|_{L^\infty(\partial D)} + \|V_0 u^i + u^i\|_{L^\infty(\partial D)}\Big)^p \|V(u^i) + u^i\|_{L^\infty(\partial D)} \\
&\leq C\|u^i\|_{L^\infty(\partial D)} + C\|\mathcal{S}\| C_g \Big(\delta + c\delta + \delta\Big)^p \|V(u^i) + u^i\|_{L^\infty(\partial D)} \\
&\leq C\|u^i\|_{L^\infty(\partial D)} + C\|\mathcal{S}\| C_g (2 + c)\delta \|V(u^i) + u^i\|_{L^\infty(\partial D)} \,,
\end{aligned}
$$

since $u^i \in \mathcal{U}_\delta$, $V(u^i) - V_0 u^i \in \mathcal{U}_\delta$ and we assume that $\delta \leq 1/(2+c)$. Provided that $C_g\delta > 0$ is sufficiently small, we obtain

$$
\|V(u^i)\|_{L^\infty(\partial D)} \leq C\|u^i\|_{L^\infty(\partial D)} \,.
$$

Utilizing the triangle inequality and the boundedness of V, it follows that

$$
\|V(u^i) + u^i\|_{L^\infty(\partial D)} \leq \|V(u^i)\|_{L^\infty(\partial D)} + \|u^i\|_{L^\infty(\partial D)} \leq C\|u^i\|_{L^\infty(\partial D)} \,,
$$

which, together with (2.41), ultimately leads to the second estimate

$$
\|V(u^i) - V_0 u^i\|_{L^\infty(\partial D)} \leq C\|\mathcal{S}\| C_g \|V(u^i) + u^i\|^{1+p}_{L^\infty(\partial D)} \leq \widetilde{C}\|u^i\|^{p+1}_{L^\infty(\partial D)} \,.
$$

□

CHAPTER 3

Domain Derivative

3.1. Variation of a Domain

With regard to iterative regularization methods for the inverse obstacle scattering problem, to which we turn in the next chapter, it is necessary to examine the differentiability of the domain-to-far-field operator. Therefore, we analyze the dependence of a solution to the scattering problem on perturbations of the underlying shape. The aim we pursue is to show the existence and representation of the domain derivative for the scattering problem (SP) using a general variational approach.

Domain or shape derivatives of solutions of boundary value problems have been used for several years in shape optimization and inverse identification problems, see, e.g., [Pir84, SZ92]. Based on the integral representation of the scattered fields, the domain derivative was formulated for acoustic scattering at an obstacle with Dirichlet boundary conditions in [KP99] and with impedance boundary conditions in [HK04]. For the exterior Helmholtz problem with a linear generalized impedance boundary condition, the domain derivative was formulated in [BCH12, Kre19]. Instead of using the representation via integral equations, the partial derivative can also be obtained by differentiating the variational formulation of the forward problem. This approach was used for Dirichlet boundary conditions in [Kir93] and was extended to Neumann and Robin boundary conditions in [Het99]. Our considerations are closely related to the ideas established in [Het22] for semilinear boundary value problems and are based on the work [FH24], in which the domain derivative for scattering problems with nonlinear impedance boundary conditions was specified.

Throughout this chapter, we assume that ∂D is of class C^4, which ensures that a solution of (2.12) lies in $H^4_{\mathrm{loc}}(\mathbb{R}^d \setminus \overline{D})$, see [BCH12]. A variation of a domain $D \subseteq B_R = \{x \in \mathbb{R}^d : |x| < R\}$ is described by a sufficiently small vector field $h \in C^1_c(B_R)$. Assuming $\|h\|_{C^1} < 1/2$ implies that h is a contraction on B_R. Thus, the vector field h defines a diffeomorphism

$$\varphi(x) = x + h(x) \quad \text{on } B_R \,. \tag{3.1}$$

We denote a perturbed domain by

$$D_h = \{x + h(x) \in \mathbb{R}^d : x \in D\}$$

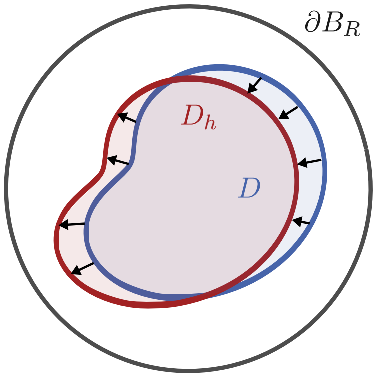

FIGURE 3.1. Scatterer D perturbed by a sufficiently small vector field h.

and set $\Omega_{R,h} = B_R \backslash \overline{D_h}$.

In order to formulate the variational formulation for the scattering problem (SP) with respect to D_h, we introduce the Sobolev space

$$V_{R,h} = \{v_h \in H^1(\Omega_{R,h}) \mid v_h|_{\partial D_h} \in H^1(\partial D_h)\}\,.$$

The corresponding scattering problem is then given by

$$\mathcal{R}_h(u_h, v_h) = (f, v_h)_{V_{R,h}} \quad \text{for all } v_h \in V_{R,h} \tag{3.2}$$

with

$$\begin{aligned}\mathcal{R}_h(u_h, v_h) &= \int_{\Omega_{R,h}} \nabla u_h \cdot \nabla \overline{v_h} - k^2 u_h \overline{v_h}\,\mathrm{d}x - \mathrm{i}k \int_{\partial D_h} \lambda u_h \overline{v_h}\,\mathrm{d}s - \mathrm{i}k \int_{\partial D_h} \mu \nabla_\tau u_h \cdot \nabla_\tau \overline{v}_h\,\mathrm{d}s \\ &\quad + \int_{\partial D_h} g(\cdot, u_h)\overline{v_h}\,\mathrm{d}s - \int_{\partial B_R} \Lambda u_h \overline{v_h}\,\mathrm{d}s\,, \\ (f, v_h)_{V_{R,h}} &= \int_{\partial B_R} \left(\frac{\partial u^i}{\partial \nu} - \Lambda u^i\right) \overline{v_h}\,\mathrm{d}s\,.\end{aligned}$$

Throughout this chapter, we consider λ, μ and g on ∂D and on perturbed boundaries ∂D_h as boundary values of functions $\lambda \in C^1(\mathbb{R}^d)$, $\mu \in C^2(\mathbb{R}^d)$ and $g\colon \mathbb{R}^d \times \mathbb{C} \to \mathbb{C}$ and assume $u \in V_R$, $u_h \in V_{R,h}$ to be the unique solutions of (2.12) and (3.2), respectively. For instance, Theorem 2.6 gives sufficient conditions on the scattering problems to be well-posed. Since u and u_h have different definition ranges, we define the function

$$\widetilde{u}_h = u_h \circ \varphi,$$

which lies in V_R if and only if $u_h \in V_{R,h}$. Furthermore, let $\widetilde{\lambda} = \lambda \circ \varphi$ and $\widetilde{\mu} = \mu \circ \varphi$. For the tangential and the normal component of a vector on the boundary ∂D we introduce the notations

$$h_\tau = \nu \times (h \times \nu) \quad \text{and} \quad h_\nu = h \cdot \nu$$

and thus $h = h_\tau + h_\nu \nu$ holds on ∂D. Additionally, the tangential gradient and the tangential divergence, defined as in Definition 2.1, can be extended to linear bounded operators

$$\nabla_\tau \colon H^{\frac{1}{2}}(\partial D) \to H^{-\frac{1}{2}}(\partial D, \mathbb{C}^d) \quad \text{and} \quad \mathrm{Div}\colon H^{\frac{1}{2}}(\partial D, \mathbb{C}^d) \to H^{-\frac{1}{2}}(\partial D),$$

see [Het99]. In the following, we denote the Jacobian matrix of the transformation φ by J_φ. The Jacobian with respect to the surface ∂D is given by

$$\mathrm{Det}(\varphi) = \sqrt{\det\left(J_{\widehat{\phi}}^\top J_{\widehat{\phi}}\right)} \Big/ \sqrt{\det\left(J_\phi^\top J_\phi\right)},$$

for local parameterizations ϕ and $\widehat{\phi} = \phi + h \circ \phi$ of ∂D and ∂D_h, respectively.

Elementary calculations show the following linearizations of the Jacobians.

Lemma 3.1. *Let $D \subseteq \mathbb{R}^d$ be a bounded domain, $\lambda \in C^1(\mathbb{R}^d, \mathbb{C})$, $\mu \in C^2(\mathbb{R}^d, \mathbb{C})$ and κ the mean curvature of ∂D. Then, for $\|h\|_{C^1} \to 0$, we have the asymptotic behavior*

$$\begin{aligned}
\|\det(J_\varphi) - 1 - \mathrm{div}(h)\|_\infty &= \mathcal{O}\left(\|h\|_{C^1}^2\right), \\
\left\|J_\varphi^{-1} J_\varphi^{-\top} \det(J_\varphi) - I + J_h + J_h^\top - \mathrm{div}(h) I\right\|_\infty &= \mathcal{O}\left(\|h\|_{C^1}^2\right), \\
\left\|\widetilde{\lambda}\mathrm{Det}(\varphi) - \lambda\left(1 + \mathrm{Div}(h_\tau) + 2\kappa h_\nu\right) - \nabla\lambda^\top h\right\|_\infty &= \mathcal{O}\left(\|h\|_{C^1}^2\right), \\
\left\|\widetilde{\mu} J_\varphi^{-1} J_\varphi^{-\top} \mathrm{Det}(\varphi) - \mu\Big((1 + \mathrm{Div}(h_\tau) + 2\kappa h_\nu) I - J_h - J_h^\top\Big) - (\nabla\mu^\top h) I\right\|_\infty &= \mathcal{O}\left(\|h\|_{C^1}^2\right).
\end{aligned}$$

Proof. For the proof of the first three identities, we refer to [Het99, Lem. 2.2, Lem. 2.17] and only address the fourth statement here.

The Jacobian matrix of $\varphi = \mathrm{id} + h$ is given by $J_\varphi = I + J_h$ and for its inverse we find $J_\varphi^{-1} = I - J_h + \mathcal{O}\left(\|h\|_{C^1}^2\right)$, since

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

Multiplying the inverse by the transposed inverse yields

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

and the Jacobian with respect to ∂D has the asymptotic behavior

$$\mathrm{Det}(\varphi) = 1 + \mathrm{Div}(h_\tau) + 2\kappa h_\nu + \mathcal{O}\left(\|h\|_{C^1}^2\right), \tag{3.3}$$

see [Het99, Lem. 2.17]. We therefore obtain

$$\begin{aligned}
J_\varphi^{-1} J_\varphi^{-\top} \mathrm{Det}(\varphi) &= \left(I - J_h - J_h^\top + \mathcal{O}\left(\|h\|_{C^1}^2\right)\right)\left(1 + \mathrm{Div}(h_\tau) + 2\kappa h_\nu + \mathcal{O}\left(\|h\|_{C^1}^2\right)\right) \\
&= I + \left(\mathrm{Div}(h_\tau) + 2\kappa h_\nu\right) I - J_h - J_h^\top + \mathcal{O}\left(\|h\|_{C^1}^2\right)
\end{aligned}$$

and with the Taylor expansion

$$\widetilde{\mu}(x) = \mu(x + h(x)) = \mu(x) + \nabla\mu^\top(x) h(x) + \mathcal{O}\left(\|h\|_{C^1}^2\right)$$

the assertion follows. □

The variational formulation (3.2) of the scattering problem with respect to D_h is defined on $V_{R,h} \times V_{R,h}$. This formulation can be pulled back to $V_R \times V_R$ by a transformation of variables with φ, i.e., we consider

$$\widetilde{\mathcal{R}}_h(u,v) = \mathcal{R}_h(u \circ \varphi^{-1}, v \circ \varphi^{-1})$$

for all $u, v \in V_R$, see [BCH11].

In order to obtain a representation of the integrals to be transformed with respect to $\Omega_{R,h}$ and ∂D_h as integrals with respect to Ω and ∂D, we have to express the basis vectors of the tangent plane to ∂D_h at a point $x_{0,h} = \varphi(x_0)$ in terms of the basis vectors of the tangent plane to ∂D at x_0. We denote by ϕ the local parameterization of the boundary ∂D. Then for a fixed point $x_0 \in \partial D$ with $\phi(0) = x_0$, the tangent vectors

$$e_i = \frac{\partial \phi(0)}{\partial x_i} \quad \text{for } i \in \{1, \dots, d-1\}$$

form a basis of the tangent plane to ∂D at x_0. Let the parameterization of the perturbed boundary ∂D_h be given by $\widehat{\phi}$ and $\{e_{h,i}\}$, $i \in \{1, \dots, d-1\}$, form the basis of the tangent plane to ∂D_h in $x_{0,h} = \varphi(x_0) = \widehat{\phi}(0)$. Using the identity $\widehat{\phi} = \varphi \circ \phi = \phi + h \circ \phi$ and the chain rule, we obtain

$$e_{h,i} = \frac{\partial \widehat{\phi}(0)}{\partial x_i} = \frac{\partial(\phi + h \circ \phi)(0)}{\partial x_i} = \frac{\partial \phi(0)}{\partial x_i} + J_h(x_0)\frac{\partial \phi(0)}{\partial x_i} = J_\varphi(x_0)\frac{\partial \phi(0)}{\partial x_i} = J_\varphi e_i \tag{3.4}$$

for $i \in \{1, \dots, d-1\}$. The corresponding covariant bases of the cotangent planes to ∂D and ∂D_h at x_0 and $x_{0,h}$ are defined by $\{e_i^*\}$ and $\{e_{h,i}^*\}$, respectively. Using (3.4) we calculate

$$e_{h,i}^* \cdot e_{h,j} = \delta_{ij} = e_i^* \cdot e_j = e_i^* \cdot J_\varphi^{-1} e_{h,j} = J_\varphi^{-\top} e_i^* \cdot e_{h,j}$$

for $i, j \in \{1, \dots, d-1\}$, where δ_{ij} denotes the Kronecker delta. Thus, we obtain the identity

$$e_{h,i}^* = J_\varphi^{-\top} e_i^*. \tag{3.5}$$

Next, we describe the surface gradient ∇_τ using the basis vectors of the cotangent plane to ∂D and ∂D_h at x_0 and $x_{0,h}$, respectively. For $w \in V_R$ and $w_h \in V_{R,h}$ we have

$$\nabla_\tau w(x_0) = \sum_{i=1}^{d-1} \frac{\partial \widehat{w}(0)}{\partial x_i} e_i^* \quad \text{and} \quad \nabla_\tau w_h(x_{0,h}) = \sum_{i=1}^{d-1} \frac{\partial \widehat{w}_h(0)}{\partial x_i} e_{h,i}^*,$$

where $\widehat{w} = w \circ \phi$ and $\widehat{w}_h = w_h \circ \widehat{\phi}$. Using the identity (3.5) and $\widehat{\phi} = \varphi \circ \phi$, we arrive at the following relation

$$\begin{aligned} \nabla_\tau(w \circ \varphi^{-1})(x_{0,h}) &= \sum_{i=1}^{d-1} \frac{\partial (w \circ \varphi^{-1} \circ \widehat{\phi})(0)}{\partial x_i} e_{h,i}^* = \sum_{i=1}^{d-1} \frac{\partial \widehat{w}(0)}{\partial x_i} e_{h,i}^* = \sum_{i=1}^{d-1} \frac{\partial \widehat{w}(0)}{\partial x_i} J_\varphi^{-\top}(x_0) e_i^* \\ &= J_\varphi^{-\top} \nabla_\tau w(x_0) \end{aligned}$$

for all $w \in V_R$. Since $x_0 \in \partial D$ was chosen arbitrarily, this result can be generalized, i.e., for all $x \in \partial D$ and $x_h \in \partial D_h$, we obtain

$$\nabla_\tau(w \circ \varphi^{-1})(x_h) = J_\varphi^{-\top} \nabla_\tau w(x) \quad \text{for } w \in V_R. \tag{3.6}$$

A transformation of variables with φ leads to

$$\begin{aligned}\widetilde{\mathcal{R}}_h(u,v) = &\int_{\Omega_R} \Big[\nabla u \cdot J_\varphi^{-1} J_\varphi^{-\top} \nabla \overline{v} - k^2 u \overline{v}\Big] \det(J_\varphi)\,\mathrm{d}x - \mathrm{i}k \int_{\partial D} \widetilde{\lambda} u \overline{v}\ \mathrm{Det}(\varphi)\,\mathrm{d}s \\ &- \mathrm{i}k \int_{\partial D} \Big[\widetilde{\mu} \nabla_\tau u \cdot J_\varphi^{-1} J_\varphi^{-\top} \nabla_\tau \overline{v}\Big]\ \mathrm{Det}(\varphi)\,\mathrm{d}s + \int_{\partial D} g(\varphi(\cdot), u) \overline{v}\ \mathrm{Det}(\varphi)\,\mathrm{d}s \\ &- \int_{\partial B_R} \Lambda u \overline{v}\,\mathrm{d}s \end{aligned} \tag{3.7}$$

for all $u, v \in V_R$. Since h is a function that has compact support in a neighborhood of ∂D, we can conclude that

$$\varphi(\partial B_R) = \partial B_R, \quad (f, v)_{V_R} = (f, v \circ \varphi^{-1})_{V_{R,h}} \quad \text{and} \quad \Lambda(v) = \Lambda(v \circ \varphi^{-1})$$

for all $v \in V_R$. Thus, we obtain that $\widetilde{u}_h = u_h \circ \varphi$ is a solution of

$$\widetilde{\mathcal{R}}_h(\widetilde{u}_h, v) = (f, v)_{V_R} \quad \text{for all } v \in V_R. \tag{3.8}$$

Note that for any perturbation h, we have the same f in (3.8) as in (2.12) given by the incident field on ∂B_R.

As in [Het22], we also have to specify assumptions on the nonlinear function g which ensure the existence of the domain derivative. We record all sufficient conditions that are applied in the subsequent considerations.

Assumption (A). A continuous function $g\colon \mathbb{R}^d \times \mathbb{C} \to \mathbb{C}$ satisfies Assumption (A), if

(i) the function g is continuously differentiable in $x \in \mathbb{R}^d$, where g satisfies the Carathéodory condition (2.14) on ∂D and on all perturbed boundaries ∂D_h as well, and similarly, its partial derivatives g_x fulfill a growth condition, i.e.,

$$|g_x(x,z)| \le |\psi_1(x)| + c_1 |z|^{p_1} \tag{3.9}$$

for almost every $x \in \partial D$ and all $z \in \mathbb{C}$. As in (2.14), we have $\psi_1 \in L^2(\partial D)$, $c_1 > 0$ and $1 \le p_1 < \infty$,

(ii) the derivatives g_z, g_{xz} exist in the sense of (2.19), i.e., for any admissible variation h, the functions $g_z(\cdot, z; w)$, $g_{xz}(\cdot, z; w) \in L^\infty(\partial D_h)$ are $\mathbb{R}$-linear functions with respect to $w \in \mathbb{C}$ and

$$\begin{aligned} g(x, z+w) - g(x,z) &= g_z(x,z;w) + o(|w|), \\ g_x(x, z+w) - g_x(x,z) &= g_{xz}(x,z;w) + o(|w|), \end{aligned} \tag{3.10}$$

for almost every $x \in \partial D_h$ and all $z, w \in \mathbb{C}$. Additionally, these derivatives also satisfy growth conditions

$$|g_z(x,z;w)|, |g_{xz}(x,z;w)| \leq (|\psi(x)| + c|z|^p)|w| \tag{3.11}$$

with corresponding functions $\psi \in L^2(\partial D),\ c > 0$ and $1 \leq p < \infty$.

The next two sections provide the results needed to indicate the existence and characterization of the domain derivative. First, we show the continuity of the solution with respect to the perturbation $h \in C^1$. Then, we prove the existence of a derivative of a solution to the scattering problem (SP) that depends linearly on h in a neighborhood of ∂D.

3.1.1. Continuous Dependence on Variations

Using Lemma 3.1 and Assumption (A), together with a localized Lipschitz-type condition on g_z, we conclude continuous dependence on variations of the domain D.

Theorem 3.2. *Let g satisfy Assumption* (A)*, and let $u \in V_R$ and $u_h \in V_{R,h}$ be the weak solutions of the well-posed scattering problems* (2.12) *and* (3.2)*, respectively. Furthermore, let $|g_z(x,z;w)| \leq \eta|w|$ for a sufficiently small constant $\eta > 0$, locally for almost every $x \in \mathcal{U}$ and for all $z \in \mathcal{V}$ in open sets $\partial D \subseteq \mathcal{U} \subseteq \mathbb{R}^d$ and $\{u(x) : x \in \partial D\} \subseteq \mathcal{V} \subseteq \mathbb{C}$. Then, the solution of the boundary value problem depends continuously on the domain D, i.e.,*

$$\lim_{\|h\|_{C^1} \to 0} \|\widetilde{u}_h - u\|_{V_R} = 0\,, \tag{3.12}$$

where the notation $\widetilde{u}_h = u_h \circ \varphi$ with $\varphi = \mathrm{id} + h$ is used.

Proof. Based on the well-posed scattering problems, the operators $T\colon V_R \to V_R$ and $T_h\colon V_R \to V_R$ given by

$$\begin{aligned} (T(w), v)_{V_R} &= \mathcal{R}(w,v) && \text{for all } v \in V_R, \\ (T_h(w), v)_{V_R} &= \widetilde{\mathcal{R}}_h(w,v) && \text{for all } v \in V_R. \end{aligned}$$

exist. Subtracting these two operators from each other and using the representation (3.7) results in

$$\begin{aligned} \|T(w) - T_h(w)\|_{V_R}^2 &= |\mathcal{R}(w, T(w) - T_h(w)) - \widetilde{\mathcal{R}}_h(w, T(w) - T_h(w))| \\ &= \Bigg| \int_{\Omega_R} \Big(\nabla w \cdot \Big[I - J_\varphi^{-1} J_\varphi^{-\top} \det(J_\varphi) \Big] \nabla \overline{(T(w) - T_h(w))} \\ &\qquad - k^2 (1 - \det(J_\varphi)) w \overline{(T(w) - T_h(w))} \Big) \,\mathrm{d}x \\ &\quad - \mathrm{i}k \int_{\partial D} (\lambda - \widetilde{\lambda} \mathrm{Det}(\varphi)) w \overline{(T(w) - T_h(w))} \,\mathrm{d}s \\ &\quad - \mathrm{i}k \int_{\partial D} \nabla_\tau w \cdot \Big[\mu I - \widetilde{\mu} J_\varphi^{-1} J_\varphi^{-\top} \mathrm{Det}(\varphi) \Big] \nabla_\tau \overline{(T(w) - T_h(w))} \,\mathrm{d}s \\ &\quad + \int_{\partial D} \Big(g(\cdot, w) - g(\varphi(\cdot), w) \mathrm{Det}(\varphi) \Big) \overline{(T(w) - T_h(w))} \,\mathrm{d}s \Bigg|. \end{aligned}$$

Estimates for the linear integrands are easily determined using the relationships from Lemma 3.1. Utilizing the asymptotic behavior of $\mathrm{Det}(\varphi)$ given in (3.3), the Mean Value Theorem, and the growth conditions (2.14) and (3.9), the expression in the last integral can be estimated by

$$\begin{aligned}
&\|g(\varphi(\cdot),w)\mathrm{Det}(\varphi)-g(\cdot,w)\|_{L^2(\partial D)}\\
&\qquad\le \|g(\varphi(\cdot),w)-g(\cdot,w)\|_{L^2(\partial D)}+\|g(\varphi(\cdot),w)(\mathrm{Div}(h_\tau)+2\kappa h_\nu)\|_{L^2(\partial D)}+\mathcal{O}(\|h\|_{C^1})\\
&\qquad\le \widehat{C}\|g_x(\cdot,w)\|_{L^2(\partial D)}\|h\|_{C^1}+\|g(\varphi(\cdot),w)(\mathrm{Div}(h_\tau)+2\kappa h_\nu)\|_{L^2(\partial D)}+\mathcal{O}(\|h\|_{C^1})\\
&\qquad\le C\left(\|\psi_1\|_{L^2(\partial D)}+\|\psi\|_{L^2(\partial D)}+\|w\|_{V_R}^{p_1}+\|w\|_{V_R}^{p}\right)\|h\|_{C^1}+\mathcal{O}(\|h\|_{C^1})
\end{aligned}$$

for constants $\widehat{C}, C>0$. Thus, for $w\in V_R$ according to Lemma 3.1 we get

$$\|T(w)-T_h(w)\|_{V_R}\le C\left(\|w\|_{V_R}+\|w\|_{V_R}^{p_1}+\|w\|_{V_R}^{p}+\|\psi_1\|_{L^2(\partial D)}+\|\psi\|_{L^2(\partial D)}\right)\|h\|_{C^1}+\mathcal{O}(\|h\|_{C^1}).$$

Due to the nonlinearity, we cannot conclude that the operators T and T_h are boundedly invertible. Therefore, we decompose the operators into their linear part, denoted by T_l and $T_{h,l}$, and their nonlinear part, denoted by T_n and $T_{h,n}$. For solutions of $T(u)=f$ and $T_h(\widetilde{u}_h)=f$, we thus obtain

$$\begin{aligned}
T_h(\widetilde{u}_h)-T_h(u)=T(u)-T_h(u)\quad&\Leftrightarrow\quad T_{h,l}(\widetilde{u}_h-u)+(T_{h,n}(\widetilde{u}_h)-T_{h,n}(u))=T(u)-T_h(u)\\
&\Leftrightarrow\quad \widetilde{u}_h-u+T_{h,l}^{-1}(T_{h,n}(\widetilde{u}_h)-T_{h,n}(u))=T_{h,l}^{-1}(T(u)-T_h(u)),
\end{aligned}$$

where

$$\begin{aligned}
(T_l(w),v)&=\int_{\Omega_R}\nabla w\cdot\nabla\overline{v}-k^2w\overline{v}\,\mathrm{d}x-\mathrm{i}k\int_{\partial D}\lambda w\overline{v}\,\mathrm{d}s-\mathrm{i}k\int_{\partial D}\mu\nabla_\tau w\cdot\nabla_\tau\overline{v}\,\mathrm{d}s-\int_{\partial B_R}\Lambda w\overline{v}\,\mathrm{d}s\,,\\
(T_n(w),v)&=\int_{\partial D}g(\cdot,w)\overline{v}\,\mathrm{d}s\,.
\end{aligned}$$

An analogous operator splitting holds for T_h. The Riesz theory at least gives us bounded invertibility of the linear operator T_l, which we can exploit to show that $T_{h,l}$ also has a bounded inverse. By the continuity of the mapping $h\mapsto T_{h,l}$ in the operator norm, and since $T_{h,l}\to T_l$ as $\|h\|_{C^1}\to 0$, the operator $T_l^{-1}(T_{h,l}-T_l)$ becomes arbitrarily small. Hence, for sufficiently small $\|h\|_{C^1}$, we can ensure $\|T_l^{-1}(T_{h,l}-T_l)\|\le\frac{1}{2}$, which allows us to apply Neumann's series to obtain

$$\|T_{h,l}^{-1}\|\le\frac{\|T_l^{-1}\|}{1-\|T_l^{-1}(T_{h,l}-T_l)\|}\le\widetilde{C}$$

for a constant $\widetilde{C}>0$, see [Kre14, Thm. 10.1]. With these considerations and (2.20), the error estimates

$$\begin{aligned}
&\|\widetilde{u}_h-u+T_{h,l}^{-1}(T_{h,n}(\widetilde{u}_h)-T_{h,n}(u))\|_{V_R}\\
&\qquad\qquad=\|T_{h,l}^{-1}(T(u)-T_h(u))\|_{V_R}\le\|T_{h,l}^{-1}\|\|T(u)-T_h(u)\|_{V_R}\\
&\qquad\qquad\le C\left(\|u\|_{V_R}+\|u\|_{V_R}^{p_1}+\|u\|_{V_R}^{p}+\|\psi_1\|_{L^2(\partial D)}+\|\psi\|_{L^2(\partial D)}\right)\|h\|_{C^1}+\mathcal{O}(\|h\|_{C^1})\\
&\qquad\qquad\le C\left(C+C^{p_1}+C^{p}+\|\psi_1\|_{L^2(\partial D)}+\|\psi\|_{L^2(\partial D)}\right)\|h\|_{C^1}+\mathcal{O}(\|h\|_{C^1})
\end{aligned}$$

and

$$
\begin{aligned}
&\|\widetilde{u}_h - u + T_{h,l}^{-1}(T_{h,n}(\widetilde{u}_h) - T_{h,n}(u))\|_{V_R} \\
&\qquad\geq \|\widetilde{u}_h - u\|_{V_R} - \|T_{h,l}^{-1}(T_{h,n}(\widetilde{u}_h) - T_{h,n}(u))\|_{V_R} \\
&\qquad\geq \|\widetilde{u}_h - u\|_{V_R} - \widetilde{C}\| \left(g(\varphi(\cdot), \widetilde{u}_h) - g(\varphi(\cdot), u)\right) \mathrm{Det}(\varphi)\|_{L^2(\partial D)} \\
&\qquad\geq \|\widetilde{u}_h - u\|_{V_R} - \widetilde{C}\|g(\varphi(\cdot), \widetilde{u}_h) - g(\varphi(\cdot), u)\|_{L^2(\partial D)} \\
&\qquad\quad - \widetilde{C}\|g(\varphi(\cdot), \widetilde{u}_h) - g(\varphi(\cdot), u)\|_{L^2(\partial D)}\mathcal{O}(\|h\|_{C^1})
\end{aligned}
$$

are valid, and it follows that

$$
\|\widetilde{u}_h - u\|_{V_R} \leq \widetilde{C}\|g(\varphi(\cdot), \widetilde{u}_h) - g(\varphi(\cdot), u)\|_{L^2(\partial D)} + \mathcal{O}(\|h\|_{C^1})\,.
$$

Furthermore,

$$
\begin{aligned}
&\|g(\varphi(x), \widetilde{u}_h(x)) - g(\varphi(x), u(x))\|_{L^2(\partial D)}^2 \\
&\qquad = \int_{\partial D} \left| \int_0^1 g_z(\varphi(x), u(x) + t(\widetilde{u}_h(x) - u(x)); \widetilde{u}_h(x) - u(x))\,\mathrm{d}t \right|^2 \mathrm{d}s \\
&\qquad \leq \int_0^1 \int_{\partial D} |g_z(\varphi(x), u(x) + t(\widetilde{u}_h(x) - u(x)); \widetilde{u}_h(x) - u(x))|^2 \,\mathrm{d}s\,\mathrm{d}t\,.
\end{aligned}
$$

Due to the assumption on g_z, we obtain

$$
\begin{aligned}
\|g(\varphi(x), \widetilde{u}_h(x)) - g(\varphi(x), u(x))\|_{L^2(\partial D)}^2 &\leq C\|g_z(\varphi(x), u(x); \widetilde{u}_h(x) - u(x))\|_{L^2(\partial D)}^2 \\
&\leq C\left(\|\psi\|_{L^2(\partial D)} + c\|u\|_{V_R}^p\right)^2 \|\widetilde{u}_h - u\|_{L^2(\partial D)}^2 \\
&\leq C\eta\|\widetilde{u}_h - u\|_{L^2(\partial D)}^2\,,
\end{aligned}
$$

which leads to

$$
(1 - C\eta)\|\widetilde{u}_h - u\|_{V_R} = \mathcal{O}(\|h\|_{C^1})\,.
$$

Thus, the solution of the boundary value problem depends continuously on the domain D if $C\eta < 1$ is satisfied. □

Note from the presented proof that assumptions on the second derivatives of g are not required for the above continuity result.

Remark 3.3. Theorem 3.2 ensures continuity of the solution with respect to domain variations, but under a locally posed condition on the derivative g_z. So far, it remains unclear how to obtain a global result without this locality assumption. ◊

For the next section, we assume the continuity of a solution to the scattering problem (SP) with respect to variations of the domain in order to show a differentiability result.

3.1.2. Differentiability

Now we consider the $\mathbb{R}$-linear boundary value problem ($\mathrm{SP}_{\mathrm{lin}}$) with g replaced by g_z. Thus, we introduce the variational problem

$$\mathcal{R}^{(\mathrm{lin})}(u,v) = (f,v)_{V_R} \quad \text{for all } v \in V_R \tag{3.13}$$

with

$$\begin{aligned}\mathcal{R}^{(\mathrm{lin})}(q,v) = &\int_{\Omega_R} \nabla q\cdot\nabla\overline{v} - k^2 q\overline{v}\,\mathrm{d}x - \mathrm{i}k\int_{\partial D}\lambda q\overline{v}\,\mathrm{d}s - \mathrm{i}k\int_{\partial D}\mu\nabla_\tau q\cdot\nabla_\tau\overline{v}\,\mathrm{d}s\\ &+\int_{\partial D} g_z(\cdot,u;q)\overline{v}\,\mathrm{d}s - \int_{\partial B_R}\Lambda q\overline{v}\,\mathrm{d}s\,.\end{aligned} \tag{3.14}$$

Using the previous considerations, we can formulate the following result regarding the existence of a derivative of the solution to the scattering problem (SP) with respect to the shape of D.

Theorem 3.4. *We assume that the boundary value problems* (2.12) *and* (3.13) *are well-posed and that the solution u of* (2.12) *is continuous with respect to the domain D in the sense of* (3.12)*. With g satisfying Assumption* (A) *the solution $u \in V_R$ is differentiable with respect to variations $h \in C_c^1(B_R)$ of the domain, i.e., there exists $w \in V_R$ that depends linearly on h with*

$$\lim_{\|h\|_{C^1}\to 0}\frac{1}{\|h\|_{C^1}}\|\widetilde{u}_h - u - w\|_{V_R} = 0\,.$$

The material derivative w is given by the unique weak solution of the $\mathbb{R}$-linear boundary value problem

$$\mathcal{R}^{(\mathrm{lin})}(w,v) = (f_h,v)_{V_R} \quad \textit{for all } v\in V_R\,, \tag{3.15}$$

where

$$\begin{aligned}(f_h,v)_{V_R} = &\int_{\Omega_R}\Big[\nabla u\cdot\Big(J_h + J_h^\top - \mathrm{div}(h)I\Big)\nabla\overline{v} + k^2\mathrm{div}(h)u\overline{v}\Big]\,\mathrm{d}x\\ &+\mathrm{i}k\int_{\partial D}\Big[\lambda(\mathrm{Div}(h_\tau)+2\kappa h_\nu)+\nabla\lambda^\top h\Big]u\overline{v}\,\mathrm{d}s\\ &+\mathrm{i}k\int_{\partial D}\nabla_\tau u\cdot\Big[\mu\Big((\mathrm{Div}(h_\tau)+2\kappa h_\nu)I - J_h - J_h^\top\Big) + (\nabla\mu^\top h)I\Big]\,\nabla_\tau\overline{v}\,\mathrm{d}s\\ &-\int_{\partial D}(\mathrm{Div}_x(g(\cdot,u)h_\tau) + 2\kappa h_\nu g(\cdot,u))\overline{v}\,\mathrm{d}s\,.\end{aligned}$$

Proof. In Section 2.4.3, we showed that the $\mathbb{R}$-linear scattering problem ($\mathrm{SP}_{\mathrm{lin}}$) is well-posed. Hence, there exists a solution $w \in V_R$ to (3.13). Since h is supported near the boundary ∂D, the function w can be extended to a radiating solution of the Helmholtz equation in the exterior domain of B_R.

The linear part of $\mathcal{R}$, defined below equation (2.12), is equal to the corresponding terms of $\mathcal{R}^{(\mathrm{lin})}$. We insert $\widetilde{u}_h - u$ in (3.14) and rewrite this expression as follows:

$$\mathcal{R}^{(\mathrm{lin})}(\widetilde{u}_h - u, v) = \mathcal{R}(\widetilde{u}_h, v) - \mathcal{R}(u,v) - \int_{\partial D}(g(\cdot,\widetilde{u}_h) - g(\cdot,u))\,\overline{v}\,\mathrm{d}s + \int_{\partial D} g_z(\cdot,u;\widetilde{u}_h - u)\overline{v}\,\mathrm{d}s$$

$$= \mathcal{R}(\widetilde{u}_h, v) - \widetilde{\mathcal{R}}_h(\widetilde{u}_h, v) - \int_{\partial D} (g(\cdot, \widetilde{u}_h) - g(\cdot, u))\, \overline{v}\, \mathrm{d}s + \int_{\partial D} g_z(\cdot, u; \widetilde{u}_h - u)\overline{v}\, \mathrm{d}s\,,$$

where we have utilized the fact that $\mathcal{R}(u, v) = \widetilde{\mathcal{R}}_h(\widetilde{u}_h, v)$, see (3.8). Now, we use the representation (3.7) for $\widetilde{\mathcal{R}}_h$ and thus obtain

$$\begin{aligned}
&\mathcal{R}^{(\mathrm{lin})}(\widetilde{u}_h - u - w, v)\\
&\quad = \int_{\Omega_R} \nabla\widetilde{u}_h \cdot \Big(I - J_\varphi^{-1} J_\varphi^{-\top} \det(J_\varphi)\Big)\nabla\overline{v} - k^2(1 - \det(J_\varphi))\widetilde{u}_h\overline{v}\, \mathrm{d}x\\
&\quad - \mathrm{i}k \int_{\partial D} \Big(\lambda - \widetilde{\lambda}\mathrm{Det}(\varphi)\Big)\, \widetilde{u}_h\overline{v}\, \mathrm{d}s - \mathrm{i}k \int_{\partial D} \nabla_\tau\widetilde{u}_h \cdot \Big(\mu I - \widetilde{\mu} J_\varphi^{-1} J_\varphi^{-\top}\mathrm{Det}(\varphi)\Big)\, \nabla_\tau\overline{v}\, \mathrm{d}s\\
&\quad + \int_{\partial D} \Big[g(\cdot, u) - g(\varphi(\cdot), \widetilde{u}_h)\mathrm{Det}(\varphi) + g_z(\cdot, u; \widetilde{u}_h - u)\Big]\, \overline{v}\, \mathrm{d}s - \mathcal{R}^{(\mathrm{lin})}(w, v)\,.
\end{aligned}$$

Next, we substitute $\mathcal{R}^{(\mathrm{lin})}(w, v)$. To do this, we use the identity specified in (3.15) and arrive at

$$\begin{aligned}
&\mathcal{R}^{(\mathrm{lin})}(\widetilde{u}_h - u - w, v)\\
&= \int_{\Omega_R} (\nabla\widetilde{u}_h - \nabla u) \cdot \Big(I - J_\varphi^{-1} J_\varphi^{-\top} \det(J_\varphi)\Big)\nabla\overline{v} - k^2(1 - \det(J_\varphi))(\widetilde{u}_h - u)\overline{v}\, \mathrm{d}x\\
&+ \int_{\Omega_R} \Big[\nabla u \cdot \Big(I - J_\varphi^{-1} J_\varphi^{-\top} \det(J_\varphi) - J_h - J_h^\top + \mathrm{div}(h) I\Big)\nabla\overline{v} - k^2(1 - \det(J_\varphi) + \mathrm{div}(h))u\overline{v}\Big]\, \mathrm{d}x\\
&- \mathrm{i}k \int_{\partial D} \Big(\lambda - \widetilde{\lambda}\mathrm{Det}(\varphi)\Big)\, (\widetilde{u}_h - u)\overline{v}\, \mathrm{d}s\\
&- \mathrm{i}k \int_{\partial D} \Big(\lambda\, (1 + \mathrm{Div}(h_\tau) + 2\kappa h_\nu) + \nabla\lambda^\top h - \widetilde{\lambda}\mathrm{Det}(\varphi)\Big)\, u\overline{v}\, \mathrm{d}s\\
&- \mathrm{i}k \int_{\partial D} \nabla_\tau(\widetilde{u}_h - u) \cdot \Big(\mu I - \widetilde{\mu} J_\varphi^{-1} J_\varphi^{-\top}\mathrm{Det}(\varphi)\Big)\, \nabla_\tau\overline{v}\, \mathrm{d}s\\
&- \mathrm{i}k \int_{\partial D} \nabla_\tau u \cdot \Big[\mu\, \Big((1 + \mathrm{Div}(h_\tau) + 2\kappa h_\nu) I - J_h - J_h^\top\Big) + \Big(\nabla\mu^\top h\Big)\, I - \widetilde{\mu} J_\varphi^{-1} J_\varphi^{-\top}\mathrm{Det}(\varphi)\Big]\, \nabla_\tau\overline{v}\, \mathrm{d}s\\
&+ \int_{\partial D} \Big[g(\cdot, u) - g(\varphi(\cdot), \widetilde{u}_h)\mathrm{Det}(\varphi) + g_z(\cdot, u; \widetilde{u}_h - u) + \mathrm{Div}_x(g(\cdot, u)h_\tau) + 2\kappa h_\nu g(\cdot, u)\Big]\, \overline{v}\, \mathrm{d}s\,.
\end{aligned}$$

Here and in the following considerations, terms on the boundary ∂D have to be understood in the duality sense of $H^{-\frac{1}{2}}$ and $H^{\frac{1}{2}}$. Using Lemma 3.1, we obtain the estimate

$$|\mathcal{R}^{(\mathrm{lin})}(\widetilde{u}_h - u - w, v)| \leq \Big(c_1\|\widetilde{u}_h - u\|_{V_R} + c_2\|u\|_{V_R} + c_3\Big)\|v\|_{V_R}\,,$$

where we still need to clarify the behavior of the constants c_1, c_2 and c_3 for $\|h\|_{C^1} \to 0$. By estimating the absolute value of the above representation of $\mathcal{R}^{(\mathrm{lin})}(\widetilde{u}_h - u - w, v)$, the first constant results in

$$\begin{aligned}
c_1 &= \Big\|I - J_\varphi^{-1} J_\varphi^{-\top} \det(J_\varphi)\Big\|_\infty + k^2\, \|1 - \det(J_\varphi)\|_\infty + |k|\, \Big\|\lambda - \widetilde{\lambda}\mathrm{Det}(\varphi)\Big\|_\infty\\
&\quad + |k|\, \Big\|\mu I - \widetilde{\mu} J_\varphi^{-1} J_\varphi^{-\top}\mathrm{Det}(\varphi)\Big\|_\infty\,.
\end{aligned}$$

Using Lemma 3.1, we conclude that $c_1 = \mathcal{O}(\|h\|_{C^1})$. However, c_1 is multiplied by $\|\widetilde{u}_h - u\|_{V_R}$ and this term is of order $o(\|h\|_{C^1})$ according to the continuity (3.12).

Furthermore, c_2 is given by

$$\begin{aligned} c_2 &= \left\| I - J_\varphi^{-1} J_\varphi^{-\top} \det(J_\varphi) - J_h - J_h^\top + \operatorname{div}(h) I \right\|_\infty + k^2 \left\| 1 - \det(J_\varphi) + \operatorname{div}(h) \right\|_\infty \\ &+ \left\| \lambda \left(1 + \operatorname{Div}(h_\tau) + 2\kappa h_\nu\right) + \nabla\lambda^\top h - \widetilde{\lambda} \operatorname{Det}(\varphi) \right\|_\infty \\ &+ \left\| \mu \left(\left(1 + \operatorname{Div}(h_\tau) + 2\kappa h_\nu\right) I - J_h - J_h^\top \right) + \left(\nabla\mu^\top h \right) I - \widetilde{\mu} J_\varphi^{-1} J_\varphi^{-\top} \operatorname{Det}(\varphi) \right\|_\infty . \end{aligned}$$

With Lemma 3.1, we again obtain $c_2 = o(\|h\|_{C^1})$.

To verify an estimate for the last integrand, we rearrange it to

$$\begin{aligned} &|g(\varphi(\cdot), \widetilde{u}_h)\operatorname{Det}(\varphi) - g(\cdot, u) - g_z(\cdot, u; \widetilde{u}_h - u) - \operatorname{Div}_x(g(\cdot, u) h_\tau) - 2\kappa h_\nu g(\cdot, u)| \\ &\quad = |g(\varphi(\cdot), \widetilde{u}_h)\operatorname{Det}(\varphi) - g(\cdot, u) - g_z(\cdot, u; \widetilde{u}_h - u) - \operatorname{Div}_x(g(\cdot, u) h_\tau) - 2\kappa h_\nu g(\cdot, u) \\ &\qquad - (g(\varphi(\cdot), \widetilde{u}_h) - g(\varphi(\cdot), \widetilde{u}_h))(1 + \operatorname{Div}(h_\tau) + 2\kappa h_\nu)| \\ &\quad \le |g(\varphi(\cdot), \widetilde{u}_h)| \, |\operatorname{Det}(\varphi) - 1 - \operatorname{Div}(h_\tau) - 2\kappa h_\nu| \\ &\qquad + |g(\varphi(\cdot), \widetilde{u}_h) - g(\cdot, u) - g_z(\cdot, u; \widetilde{u}_h - u) + g(\varphi(\cdot), \widetilde{u}_h)\operatorname{Div}(h_\tau) \\ &\qquad - \operatorname{Div}_x(g(\cdot, u) h_\tau) + 2\kappa h_\nu g(\varphi(\cdot), \widetilde{u}_h) - 2\kappa h_\nu g(\cdot, u)| . \end{aligned}$$

In the first line, we can apply (2.14) and Lemma 3.1. By adding and subtracting further terms, it follows

$$\begin{aligned} &|g(\varphi(\cdot), \widetilde{u}_h)\operatorname{Det}(\varphi) - g(\cdot, u) - g_z(\cdot, u; \widetilde{u}_h - u) - \operatorname{Div}_x(g(\cdot, u) h_\tau) - 2\kappa h_\nu g(., u)| \\ &\quad \le (|\psi_0(\varphi(\cdot))| + c_0 |\widetilde{u}_h|^p) \, o(\|h\|_{C^1}) \\ &\qquad + |g(\varphi(\cdot), \widetilde{u}_h) - g(\cdot, u) - g_z(\cdot, u; \widetilde{u}_h - u) + g(\varphi(\cdot), \widetilde{u}_h)\operatorname{Div}(h_\tau) \\ &\qquad - \operatorname{Div}_x(g(\cdot, u) h_\tau) + 2\kappa h_\nu g(\varphi(\cdot), \widetilde{u}_h) - 2\kappa h_\nu g(\cdot, u) \\ &\qquad - (g(\cdot, \widetilde{u}_h) - g(\cdot, \widetilde{u}_h))(1 + \operatorname{Div}(h_\tau) + 2\kappa h_\nu) - (g_x(\cdot, \widetilde{u}_h) - g_x(\cdot, \widetilde{u}_h)) h_\tau| \\ &\quad \le (|\psi_0(\varphi(\cdot))| + c_0 |\widetilde{u}_h|^p) o(\|h\|_{C^1}) + |g(\varphi(\cdot), \widetilde{u}_h) - g(\cdot, \widetilde{u}_h) - g_x(\cdot, \widetilde{u}_h) \, h_\tau| \\ &\qquad + |g(\cdot, \widetilde{u}_h) - g(\cdot, u) - g_z(\cdot, u; \widetilde{u}_h - u)| + | \left(g(\varphi(\cdot), \widetilde{u}_h) - g(\cdot, \widetilde{u}_h)\right) \operatorname{Div}(h_\tau)| \\ &\qquad + | \left(g(\cdot, \widetilde{u}_h) - g(\cdot, u)\right) \operatorname{Div}(h_\tau)| + | \left(g_x(\cdot, \widetilde{u}_h) - g_x(\cdot, u)\right) h_\tau| \\ &\qquad + | \left(g(\varphi(\cdot), \widetilde{u}_h) - g(\cdot, \widetilde{u}_h)\right) 2\kappa h_\nu| + | \left(g(\cdot, \widetilde{u}_h) - g(\cdot, u)\right) 2\kappa h_\nu| . \end{aligned}$$

Using the growth conditions from Assumption (A), the continuity of the Nemytskii operator, and the continuity of solutions with respect to h, we obtain

$$\begin{aligned} c_3 &= \|g(\varphi(\cdot), \widetilde{u}_h)\operatorname{Det}(\varphi) - g(\cdot, u) - g_z(\cdot, u; \widetilde{u}_h - u) - \operatorname{Div}_x(g(\cdot, u) h_\tau) - 2\kappa h_\nu g(\cdot, u)\|_{L^2(\partial D)} \\ &\le (\|\psi\|_{L^2} + C) o(\|h\|_{C^1}) . \end{aligned}$$

Finally, the Riesz representation theorem (see [Kre14, Thm. 4.10]) implies that $\widetilde{u}_h - u - w \in V_R$ is the unique solution of

$$\mathcal{R}^{(\mathrm{lin})}(\widetilde{u}_h - u - w, v) = (l_h, v)_{V_R}$$

for all $v \in V_R$ with a functional $l_h \in V_R$ satisfying $\|l_h\|_{V_R} = o(\|h\|_{C^1})$. Due to the well-posedness of (3.13), we conclude

$$\frac{1}{\|h\|_{C^1}}\|\widetilde{u}_h - u - w\|_{V_R} \leq \frac{c\,\|l_h\|_{V_R}}{\|h\|_{C^1}} \longrightarrow 0 \quad \text{for } \|h\|_{C^1} \to 0.$$

□

Note that the material derivative $w \in V_R$ depends linearly on h in a neighborhood of the boundary ∂D. Therefore, the material derivative itself is not an appropriate representation of the derivative. What we are interested in is a domain derivative that depends only on h at the boundary ∂D and is a radiating solution of the Helmholtz equation.

3.2. Shape Derivative

As known from shape derivatives for linear boundary value problems, the material derivative can be read in the sense of the chain rule, which leads to the notion of the domain derivative u'.

Now the domain $D \subseteq \mathbb{R}^d$ has the regularity $\partial D \in C^{3,\alpha}$. This ensures that the solution u of (2.12) lies in $H^3_{\mathrm{loc}}(\mathbb{R}^d \backslash \overline{D})$ and $\nabla_\tau u \in H^{\frac{3}{2}}(\partial D)$. Consequently, the domain derivative u' given in the following theorem lies in the Hilbert space V_R.

Theorem 3.5. *The material derivative defined in Theorem 3.4 has the form $w = u' + \nabla u \cdot h$, where $u \in H^3(B_R\backslash\overline{D})$ denotes the solution of* (2.12) *and the domain derivative $u' \in V_R$ is the unique weak solution of the $\mathbb{R}$-linear boundary value problem*

$$\Delta u' + k^2 u' = 0 \quad \textit{in } \Omega_R, \tag{3.16}$$

together with

$$\begin{aligned}\frac{\partial u'}{\partial \nu} &+ \mathrm{i}k\Big(\lambda u' - \mathrm{Div}(\mu \nabla_\tau u')\Big) - g_z(\cdot, u; u') \\ &= \mathrm{Div}(h_\nu \nabla_\tau u) + k^2 u h_\nu - \mathrm{i}k\lambda\left(2\kappa u h_\nu + \frac{\partial u}{\partial \nu} h_\nu\right) - \mathrm{i}k\frac{\partial \lambda}{\partial \nu} u h_\nu \\ &\quad + \mathrm{i}k\mathrm{Div}\left(h_\nu\left(2\mu\kappa + \frac{\partial \mu}{\partial \nu} - 2\mu J_\nu\right)\nabla_\tau u\right) + \mathrm{i}k\mathrm{Div}\left(\mu\nabla_\tau\left(\frac{\partial u}{\partial \nu}h_\nu\right)\right) \\ &\quad + g_z\left(\cdot, u; \frac{\partial u}{\partial \nu}h_\nu\right) + 2\kappa g(\cdot, u) h_\nu\end{aligned} \tag{3.17}$$

on ∂D and

$$\frac{\partial u'}{\partial \nu} = \Lambda u' \quad \textit{on } \partial B_R\,. \tag{3.18}$$

Here, the boundary condition on ∂B_R ensures that u' can be uniquely extended to a weak radiating solution of the Helmholtz equation in $\mathbb{R}^d\backslash\overline{D}$.

Proof. From Green's representation theorem (see [CK13, Thm. 2.1]) and the Sommerfeld radiation condition (2.6) we obtain

$$u^s = \mathrm{DL}u + \mathrm{SL}\left(\mathrm{i}k\Big(\lambda u - \mathrm{Div}(\mu\nabla_\tau u)\Big) - g(\cdot, u)\right) \quad \text{in } \Omega_R.$$

Thus, the mapping properties of the potentials DL: $H^{\frac{1}{2}}(\partial D) \to H^2(\Omega_R)$ and SL: $H^{-\frac{1}{2}}(\partial D) \to H^2(\Omega_R)$, if ∂D is C^2, leads to $u \in H^2(\Omega_R)$, see [McL00, p.210 ff.]. Therefore, the trace of $h \cdot \nabla u$ can be considered in $H^{\frac{1}{2}}(\partial D)$ and $H^{-\frac{1}{2}}(\partial D)$.

Section 2.4.3 ensures the existence of a solution $u' \in V_R$ to the given scattering problem, and Theorem 3.4 provides the existence of a material derivative $w \in V_R$ defined by (3.15). It therefore remains to prove the decomposition $w = u' + h \cdot \nabla u$. Inserting $h \cdot \nabla u - w$ in (3.14) results in

$$\begin{aligned} \mathcal{R}^{(\mathrm{lin})}(h \cdot \nabla u - w, v) &= \mathcal{R}^{(\mathrm{lin})}(h \cdot \nabla u, v) - \mathcal{R}^{(\mathrm{lin})}(w, v) \\ &= \int_{\Omega_R} \nabla(h \cdot \nabla u) \cdot \nabla \overline{v} - k^2 (h \cdot \nabla u) \overline{v} \,\mathrm{d}x - \int_{\partial B_R} \Lambda(h \cdot \nabla u) \overline{v} \,\mathrm{d}s \\ &\quad - \int_{\Omega_R} \nabla w \cdot \nabla \overline{v} - k^2 w \overline{v} \,\mathrm{d}x + \int_{\partial B_R} \Lambda w \overline{v} \,\mathrm{d}s + \mathcal{I}\,, \end{aligned} \tag{3.19}$$

where $\mathcal{I}$ denotes the sum of boundary integrals over ∂D, which will be specified later. Since h is compactly supported in a neighborhood of ∂D, we can conclude that $\langle \Lambda(h \cdot \nabla u), v \rangle_{\partial B_R}$ vanishes. The product rule leads to the relation

$$\begin{aligned} \nabla u \cdot \Big(J_h + J_h^\top - \mathrm{div}(h) I\Big) \nabla v = \mathrm{div}\Big((h \cdot \nabla u)\nabla v + (h \cdot \nabla v)\nabla u - (\nabla u \cdot \nabla v) h\Big) \\ - (h \cdot \nabla u)\mathrm{div}(\nabla v) - (h \cdot \nabla v)\mathrm{div}(\nabla u)\,, \end{aligned}$$

and by rearranging the terms, we obtain

$$\begin{aligned} \int_{\Omega_R} \nabla(h \cdot \nabla u) \cdot \nabla \overline{v} \,\mathrm{d}x = \int_{\Omega_R} \Big[\nabla u \cdot \Big(J_h + J_h^\top - \mathrm{div}(h) I\Big) \nabla \overline{v} + (h \cdot \nabla \overline{v})\mathrm{div}(\nabla u) \\ - \mathrm{div}\Big((h \cdot \nabla \overline{v})\nabla u - (\nabla u \cdot \nabla \overline{v}) h\Big)\Big] \,\mathrm{d}x\,. \end{aligned}$$

Inserting this identity into (3.19) leads to

$$\begin{aligned} \mathcal{R}^{(\mathrm{lin})}(h \cdot \nabla u - w, v) = \int_{\Omega_R} \Big[\nabla u \cdot \Big(J_h + J_h^\top - \mathrm{div}(h) I\Big) \nabla \overline{v} + (h \cdot \nabla \overline{v})\mathrm{div}(\nabla u) \\ - \mathrm{div}\Big((h \cdot \nabla \overline{v})\nabla u - (\nabla u \cdot \nabla \overline{v}) h\Big) - k^2 (h \cdot \nabla u)\overline{v}\Big] \,\mathrm{d}x \\ - \int_{\Omega_R} \nabla w \cdot \nabla \overline{v} - k^2 w \overline{v} \,\mathrm{d}x + \int_{\partial B_R} \Lambda w \overline{v} \,\mathrm{d}s + \mathcal{I}\,. \end{aligned}$$

For the material derivative w we use the representation (3.15) to replace $\mathcal{R}^{(\mathrm{lin})}(w, v)$, which removes the first term and we thus arrive at

$$\begin{aligned} &\mathcal{R}^{(\mathrm{lin})}(h \cdot \nabla u - w, v) \\ &= \int_{\Omega_R} \Big[\nabla u \cdot \Big(J_h + J_h^\top - \mathrm{div}(h) I\Big) \nabla \overline{v} + (h \cdot \nabla \overline{v})\mathrm{div}(\nabla u) - \mathrm{div}\Big((h \cdot \nabla \overline{v})\nabla u - (\nabla u \cdot \nabla \overline{v}) h\Big) \\ &\qquad - k^2 (h \cdot \nabla u)\overline{v}\Big] \,\mathrm{d}x - \int_{\Omega_R} \Big[\nabla u \cdot \Big(J_h + J_h^\top - \mathrm{div}(h) I\Big) \nabla \overline{v} + k^2 u \overline{v} \mathrm{div}(h)\Big] \,\mathrm{d}x \\ &\quad + \mathcal{I}_\lambda + \mathcal{I}_\mu + \mathcal{I}_g \end{aligned}$$

$$
\begin{aligned}
&= -\int_{\Omega_R} \Big[k^2(h\cdot\nabla u)\overline{v} - \underbrace{\operatorname{div}(\nabla u)}_{=-k^2u}(h\cdot\nabla\overline{v}) + k^2u\overline{v}\operatorname{div}(h) - \operatorname{div}\Big((h\cdot\nabla\overline{v})\nabla u - (\nabla u\cdot\nabla\overline{v})h\Big)\Big]\,\mathrm{d}x \\
&\quad + \mathcal{I}_\lambda + \mathcal{I}_\mu + \mathcal{I}_g \\
&= -\int_{\Omega_R} \Big[\underbrace{k^2(h\cdot\nabla u)\overline{v} + k^2u(h\cdot\nabla\overline{v}) + k^2u\overline{v}\operatorname{div}(h)}_{=\operatorname{div}(k^2u\overline{v}h)} + \operatorname{div}\Big((h\cdot\nabla\overline{v})\nabla u - (\nabla u\cdot\nabla\overline{v})h\Big)\Big]\,\mathrm{d}x \\
&\quad + \mathcal{I}_\lambda + \mathcal{I}_\mu + \mathcal{I}_g \\
&= -\int_{\Omega_R} \operatorname{div}\Big((h\cdot\nabla\overline{v})\nabla u - (\nabla u\cdot\nabla\overline{v})h + k^2u\overline{v}h\Big)\,\mathrm{d}x + \mathcal{I}_\lambda + \mathcal{I}_\mu + \mathcal{I}_g\,,
\end{aligned}
$$

where the boundary integrals $\mathcal{I}_\lambda$, $\mathcal{I}_\mu$ and $\mathcal{I}_g$ are given by

$$
\begin{aligned}
\mathcal{I}_\lambda &= -\mathrm{i}k\int_{\partial D}\lambda(h\cdot\nabla u)\overline{v}\,\mathrm{d}s - \mathrm{i}k\int_{\partial D}\Big(\lambda\big(\operatorname{Div}(h_\tau) + 2\kappa h_\nu\big) + \nabla\lambda^\top h\Big)u\overline{v}\,\mathrm{d}s\,, \\
\mathcal{I}_\mu &= -\mathrm{i}k\int_{\partial D}\mu\nabla_\tau(h\cdot\nabla u)\cdot\nabla_\tau\overline{v}\,\mathrm{d}s \\
&\qquad - \mathrm{i}k\int_{\partial D}\nabla_\tau u\cdot\Big[\mu\Big((\operatorname{Div}(h_\tau) + 2\kappa h_\nu)I - J_h - J_h^\top\Big) + (\nabla\mu^\top h)I\Big]\,\nabla_\tau\overline{v}\,\mathrm{d}s\,, \\
\mathcal{I}_g &= \int_{\partial D} g_z(\cdot,u;h\cdot\nabla u)\overline{v}\,\mathrm{d}s + \int_{\partial D}\Big(\operatorname{Div}_x\big(g(\cdot,u)h_\tau\big) + 2\kappa h_\nu g(\cdot,u)\Big)\overline{v}\,\mathrm{d}s\,.
\end{aligned}
$$

Using Gauss's divergence theorem (see [KH15, Thm. A.11]), the volume integral over the divergence can be replaced by a surface integral. By exploiting the compactness of the support of h in B_R, we obtain

$$
\begin{aligned}
&\mathcal{R}^{(\mathrm{lin})}(h\cdot\nabla u - w, v) \\
&\qquad = -\int_{\partial\Omega_R}\nu\cdot\Big((h\cdot\nabla\overline{v})\nabla u - (\nabla u\cdot\nabla\overline{v})h + k^2u\overline{v}h\Big)\,\mathrm{d}s + \mathcal{I}_\lambda + \mathcal{I}_\mu + \mathcal{I}_g \\
&\qquad = \int_{\partial D}\nu\cdot\Big((h\cdot\nabla\overline{v})\nabla u - (\nabla u\cdot\nabla\overline{v})h + k^2u\overline{v}h\Big)\,\mathrm{d}s + \mathcal{I}_\lambda + \mathcal{I}_\mu + \mathcal{I}_g \\
&\qquad = \int_{\partial D}\Big[(h\cdot\nabla\overline{v})(\nabla u\cdot\nu) - (\nabla u\cdot\nabla\overline{v})h_\nu + k^2u\overline{v}h_\nu\Big]\,\mathrm{d}s + \mathcal{I}_\lambda + \mathcal{I}_\mu + \mathcal{I}_g\,.
\end{aligned}
$$

Now we are looking for a suitable representation of the boundary integrals to show the validity of

$$
\mathcal{R}^{(\mathrm{lin})}(h\cdot\nabla u - w, v) = -\mathcal{R}^{(\mathrm{lin})}(u', v)\,.
$$

Applying the product rule for the surface divergence operator leads to

$$
\begin{aligned}
\operatorname{Div}(\lambda uvh_\tau) &= \lambda\operatorname{Div}(h_\tau)uv + \nabla_\tau(\lambda uv)\cdot h_\tau = \lambda\operatorname{Div}(h_\tau)uv + \nabla(\lambda uv)\cdot h - \nabla(\lambda uv)_\nu h_\nu \\
&= \lambda\operatorname{Div}(h_\tau)uv + \nabla\lambda^\top huv + \lambda(h\cdot\nabla u)v + \lambda u(h\cdot\nabla v) - \frac{\partial\lambda}{\partial\nu}uh_\nu v - \lambda\frac{\partial u}{\partial\nu}h_\nu v \\
&\quad - \lambda u(\nabla v\cdot\nu)h_\nu\,.
\end{aligned}
$$

Therefore, we obtain

$$\mathcal{I}_\lambda = -\mathrm{i}k \int_{\partial D} 2\kappa h_\nu u\overline{v} + \frac{\partial \lambda}{\partial \nu} u h_\nu \overline{v} + \lambda \frac{\partial u}{\partial \nu} h_\nu \overline{v} - \lambda u (h\cdot \nabla \overline{v}) + \lambda u (\nabla \overline{v}\cdot \nu) h_\nu \,\mathrm{d}s\,,$$

where we have used that the integral over $\mathrm{Div}(\lambda u v h_\tau)$ vanishes, see, e.g., [Het99, Lem. 2.4]. With the boundary integral $\mathcal{I}_\mu$ we proceed similarly as for $\mathcal{I}_\lambda$. Applying the product rule for the surface divergence leads to

$$\begin{aligned}\mathrm{Div}\Big(\mu(\nabla_\tau u\cdot\nabla_\tau v)h_\tau\Big) &= \mu\nabla_\tau u\cdot\nabla_\tau v\mathrm{Div}(h_\tau) + \nabla_\tau(\mu\nabla_\tau u\cdot\nabla_\tau v)\cdot h_\tau \\ &= \nabla_\tau u\cdot\Big[\mu\mathrm{Div}(h_\tau) + \nabla_\tau\mu^\top h_\tau\Big] I\nabla_\tau v + \mu\nabla_\tau(\nabla_\tau u\cdot\nabla_\tau v)\cdot h_\tau\,.\end{aligned} \tag{3.20}$$

In order to obtain a convenient representation for the last term, we need a C^1-extension of $\nabla_\tau u$, i.e., a C^2-extension of u to the boundary ∂D, as well as a C^1-extension of ν. With Definition 2.1 we have

$$\nabla_\tau(\nabla_\tau u) = \nu\times(\widetilde{\nabla_\tau u}\times\nu), \quad \text{where} \quad \widetilde{\nabla_\tau u} = \widetilde{\nu}\times(\nabla\widetilde{\widetilde{u}}\times\widetilde{\nu})$$

for $\widetilde{\widetilde{u}}\in C^2(\Omega_R)$ and $\widetilde{\nu}\in C^1(\Omega_R)$, $\|\widetilde{\nu}\|=1$. In the following, we write u instead of $\widetilde{\widetilde{u}}$. If we use the same identity for v, we obtain

$$\begin{aligned}\nabla_\tau(\nabla_\tau u\cdot\nabla_\tau v)\cdot h_\tau = \nabla(\widetilde{\nabla_\tau u}\cdot\widetilde{\nabla_\tau v})\cdot h_\tau &= (J^\top_{\widetilde{\nabla_\tau u}}\nabla_\tau v + J^\top_{\widetilde{\nabla_\tau v}}\nabla_\tau u)\cdot h_\tau \\ &= J_{\widetilde{\nabla_\tau u}} h_\tau\cdot\nabla_\tau v + \nabla_\tau u\cdot J_{\widetilde{\nabla_\tau v}} h_\tau\,.\end{aligned} \tag{3.21}$$

Further, there holds

$$\nabla_\tau(h\cdot\nabla_\tau u)\cdot\nabla_\tau v = \nabla_\tau u\cdot J_h\nabla_\tau v + J^\top_{\widetilde{\nabla_\tau u}} h_\tau\cdot\nabla_\tau v + h_\nu J^\top_{\widetilde{\nabla_\tau u}}\nu\cdot\nabla_\tau v\,.$$

This result applies analogously to reversed roles of u and v. Subtracting and adding the terms $\nabla_\tau(h\cdot\nabla_\tau u)\cdot\nabla_\tau v$ and $\nabla_\tau u\cdot\nabla_\tau(h\cdot\nabla_\tau v)$ in (3.21) leads to

$$\begin{aligned}\nabla_\tau(\nabla_\tau u\cdot\nabla_\tau v)\cdot h_\tau = &\Big(J_{\widetilde{\nabla_\tau u}} - J^\top_{\widetilde{\nabla_\tau u}}\Big)h_\tau\cdot\nabla_\tau v + \nabla_\tau u\cdot\Big(J_{\widetilde{\nabla_\tau v}} - J^\top_{\widetilde{\nabla_\tau v}}\Big)h_\tau - h_\nu J^\top_{\widetilde{\nabla_\tau u}}\nu\cdot\nabla_\tau v \\ &- \nabla_\tau u\cdot h_\nu J^\top_{\widetilde{\nabla_\tau v}}\nu - \nabla_\tau u\cdot(J_h + J_h^\top)\nabla_\tau v + \nabla_\tau(h\cdot\nabla_\tau u)\cdot\nabla_\tau v \\ &+ \nabla_\tau u\cdot\nabla_\tau(h\cdot\nabla_\tau v)\,.\end{aligned} \tag{3.22}$$

Moreover, we have that

$$\Big(J_{\widetilde{\nabla_\tau u}} - J^\top_{\widetilde{\nabla_\tau u}}\Big)h_\tau = \mathrm{curl}(\widetilde{\nabla_\tau u})\times h_\tau$$

and

$$\nu\cdot\mathrm{curl}(\widetilde{\nabla_\tau u}) = \nu\cdot\mathrm{curl}(\widetilde{\nu}\times(\nabla u\times\widetilde{\nu})) = \mathrm{Div}(\nabla u\times\nu) = \nu\cdot\mathrm{curl}(\nabla u) = 0\,,$$

see [KH15, Lem. A.18]. This means that $\mathrm{curl}(\widetilde{\nabla_\tau u})$ has a contribution to the normal direction and is thus tangential to ∂D. Therefore, the cross product $\mathrm{curl}(\widetilde{\nabla_\tau u})\times h_\tau$ points in normal direction and we obtain

$$\Big(J_{\widetilde{\nabla_\tau u}} - J^\top_{\widetilde{\nabla_\tau u}}\Big)h_\tau\cdot\nabla_\tau v = 0.$$

From $\nabla_\tau u \cdot \nu = 0$ on ∂D, we arrive at

$$0 = \nabla_\tau(\nabla_\tau u \cdot \nu) \cdot \nabla_\tau v = \nabla(\widetilde{\nabla_\tau u} \cdot \nu) \cdot \nabla_\tau v = \Big(J^\top_{\widetilde{\nabla_\tau u}} \nu + J_\nu^\top \nabla_\tau u \Big) \cdot \nabla_\tau v\,. \tag{3.23}$$

If we swap the roles of u and v, we receive analogous statements for $\nabla_\tau v$ or $\widetilde{\nabla_\tau v}$. With (3.23) we get the identities

$$-J^\top_{\widetilde{\nabla_\tau u}} \nu \cdot \nabla_\tau v = J_\nu^\top \nabla_\tau u \cdot \nabla_\tau v \quad \text{and} \quad - \nabla_\tau u \cdot J^\top_{\widetilde{\nabla_\tau v}} \nu = \nabla_\tau u \cdot J_\nu^\top \nabla_\tau v$$

and we therefore obtain

$$-h_\nu J^\top_{\widetilde{\nabla_\tau u}} \nu \cdot \nabla_\tau v - \nabla_\tau u \cdot h_\nu J^\top_{\widetilde{\nabla_\tau v}} \nu = \nabla_\tau u \cdot h_\nu (J_\nu + J_\nu^\top) \nabla_\tau v = \nabla_\tau u \cdot 2 h_\nu J_\nu \nabla_\tau v\,,$$

where in the last step we utilized the fact that the curvature operator J_ν is symmetric, see [Hag19, Lem. 3.11].

Inserting the above considerations in (3.22) leads to

$$\begin{aligned} \nabla_\tau(\nabla_\tau u \cdot \nabla_\tau v) \cdot h_\tau = \nabla_\tau u \cdot \Big[2 h_\nu J_\nu - \big(J_h + J_h^\top\big)\Big] \nabla_\tau v + \nabla_\tau (h \cdot \nabla_\tau u) \cdot \nabla_\tau v \\ + \nabla_\tau u \cdot \nabla_\tau (h \cdot \nabla_\tau v)\,. \end{aligned}$$

For the surface divergence of the term $\mu(\nabla_\tau u \cdot \nabla_\tau v) h_\tau$, we find

$$\begin{aligned} \mathrm{Div}\Big(\mu(\nabla_\tau u \cdot \nabla_\tau v) h_\tau\Big) &= \nabla_\tau u \cdot \Big[\Big(\mu \mathrm{Div}(h_\tau) + \nabla_\tau \mu^\top h_\tau \Big) I + 2\mu h_\nu J_\nu - \mu (J_h + J_h^\top) \Big] \nabla_\tau v \\ &\quad + \mu \nabla_\tau (h \cdot \nabla_\tau u) \cdot \nabla_\tau v + \mu \nabla_\tau u \cdot \nabla_\tau (h \cdot \nabla_\tau v) \\ &= \nabla_\tau u \cdot \left[\left(\mu \mathrm{Div}(h_\tau) + \nabla \mu^\top h - \frac{\partial \mu}{\partial \nu} h_\nu \right) I + 2\mu h_\nu J_\nu - \mu (J_h + J_h^\top) \right] \nabla_\tau v \\ &\quad + \mu \nabla_\tau (h \cdot \nabla u) \cdot \nabla_\tau v + \mu \nabla_\tau u \cdot \nabla_\tau (h \cdot \nabla v) \\ &\quad - \mu \nabla_\tau (\nabla u \cdot \nu) h_\nu \cdot \nabla_\tau v - \mu \nabla_\tau u \cdot \nabla_\tau (\nabla v \cdot \nu) h_\nu\,, \end{aligned}$$

which provides the relation

$$\begin{aligned} \mathcal{I}_\mu = -\mathrm{i}k \int_{\partial D} \nabla_\tau u \cdot \left[\left(2\mu\kappa h_\nu + \frac{\partial \mu}{\partial \nu} h_\nu \right) I - 2\mu h_\nu J_\nu \right] \nabla_\tau \overline{v} + \mu \nabla_\tau \left(\frac{\partial u}{\partial \nu} h_\nu \right) \cdot \nabla_\tau \overline{v} \,\mathrm{d}s \\ - \mathrm{i}k \int_{\partial D} \mathrm{Div}(\mu \nabla_\tau u)(h \cdot \nabla \overline{v}) - \mathrm{Div}(\mu \nabla_\tau u) \left((\nabla \overline{v} \cdot \nu) h_\nu \right) \,\mathrm{d}s\,. \end{aligned}$$

Finally, for the last boundary integral regarding the nonlinearity g, we use the identity

$$\begin{aligned} \mathrm{Div}(g(\cdot,u) h_\tau v) &= \mathrm{Div}_x(g(\cdot,u) h_\tau) v + g_z(\cdot, u; h_\tau \cdot \nabla u) v + g(\cdot,u)(h_\tau \cdot \nabla_{\partial D} v) \\ &= \mathrm{Div}_x(g(\cdot,u) h_\tau) v + g_z(\cdot, u; h_\tau \cdot \nabla u) v + g(\cdot,u)(h \cdot \nabla v) - g(\cdot,u)(\nabla v \cdot \nu) h_\nu \end{aligned}$$

and therefore we receive

$$\mathcal{I}_g = \int_{\partial D} g_z \left(\cdot, u; \frac{\partial u}{\partial \nu} h_\nu \right) \overline{v} + 2\kappa h_\nu g(\cdot,u) \overline{v} - g(\cdot,u)(h \cdot \nabla \overline{v}) + g(\cdot,u)(\nabla \overline{v} \cdot \nu) h_\nu \,\mathrm{d}s\,.$$

In the representations of the boundary integrals, one term with $(h \cdot \overline{v})$ and one term with $(\nabla\overline{v}\cdot\nu)h_\nu$ appear. By combining these and inserting the boundary condition (2.11), we arrive at

$$
\begin{aligned}
-\int_{\partial D}\Big[-\mathrm{i}k\lambda u + \mathrm{i}k\mathrm{Div}(\mu\nabla_\tau u) + g(\cdot,u)\Big]\Big((h\cdot\nabla\overline{v}) - (\nabla\overline{v}\cdot\nu)h_\nu\Big)\,\mathrm{d}s \\
= -\int_{\partial D}(\nabla u\cdot\nu)(h\cdot\nabla\overline{v}) - (\nabla u\cdot\nu)(\nabla\overline{v}\cdot\nu)h_\nu\,\mathrm{d}s\,.
\end{aligned}
$$

With

$$
\int_{\partial D}\Big[(\nabla u\cdot\nu)(\nabla\overline{v}\cdot\nu) - (\nabla u\cdot\nabla\overline{v})\Big]h_\nu = -\int_{\partial D} h_\nu\nabla_\tau u\cdot\nabla_\tau\overline{v}\,\mathrm{d}s\,,
$$

we finally obtain

$$
\begin{aligned}
-\mathcal{R}^{(\mathrm{lin})}(u',v) &= \mathcal{R}^{(\mathrm{lin})}(h\cdot\nabla u - w, v) \\
&= -\int_{\partial D}\Big[\nabla_\tau u\cdot\nabla_\tau\overline{v} - k^2u\overline{v}\Big]h_\nu\,\mathrm{d}s - \mathrm{i}k\int_{\partial D}2\kappa h_\nu u\overline{v} + \frac{\partial\lambda}{\partial\nu}uh_\nu\overline{v} + \lambda\frac{\partial u}{\partial\nu}h_\nu\overline{v}\,\mathrm{d}s \\
&\quad - \mathrm{i}k\int_{\partial D}\nabla_\tau u\cdot\left[\left(2\mu\kappa h_\nu + \frac{\partial\mu}{\partial\nu}h_\nu\right)I - 2\mu h_\nu J_\nu\right]\nabla_\tau\overline{v} + \mu\nabla_\tau\left(\frac{\partial u}{\partial\nu}h_\nu\right)\cdot\nabla_\tau\overline{v}\,\mathrm{d}s \\
&\quad + \int_{\partial D} g_z\left(\cdot,u;\frac{\partial u}{\partial\nu}h_\nu\right)\overline{v} + 2\kappa h_\nu g(\cdot,u)\overline{v}\,\mathrm{d}s\,.
\end{aligned}
$$

Thus, u' can be extended in $\mathbb{R}^d\backslash\overline{D}$ to the weak scattered solution of (3.16)–(3.18). □

Note that the domain derivative depends only on the normal component of h at the boundary ∂D. Furthermore, the domain derivative u' solves an $\mathbb{R}$-linear problem which has the same form as ($\mathrm{SP}_{\mathrm{lin}}$), but with a different right-hand side in the boundary condition. This in turn means that (2.29) gives an integral equation formulation equivalent to (3.16)–(3.18) by replacing f with

$$
\begin{aligned}
\hat{f} = \mathrm{Div}(h_\nu\nabla_\tau u) &+ k^2uh_\nu - \mathrm{i}k\lambda\left(2\kappa uh_\nu + \frac{\partial u}{\partial\nu}h_\nu\right) - \mathrm{i}k\frac{\partial\lambda}{\partial\nu}uh_\nu \\
&+ \mathrm{i}k\mathrm{Div}\left(h_\nu\left(2\mu\kappa + \frac{\partial\mu}{\partial\nu} - 2\mu J_\nu\right)\nabla_\tau u\right) + \mathrm{i}k\mathrm{Div}\left(\mu\nabla_\tau\left(\frac{\partial u}{\partial\nu}h_\nu\right)\right) \\
&+ g_z\left(\cdot,u;\frac{\partial u}{\partial\nu}h_\nu\right) + 2\kappa g(\cdot,u)h_\nu\,.
\end{aligned}
$$

CHAPTER 4

Shape Reconstruction

The shape reconstruction of a scattering object D from the knowledge of the far-field pattern for all observation directions and for one or more incident directions with fixed wave number k is called the inverse obstacle scattering problem. Notably, the inverse scattering problem is nonlinear in the sense that the scattered wave depends nonlinearly on the scatterer. Moreover, the determination of D does not continuously depend on the far-field pattern in a reasonable norm. The nonlinearity and the ill-posedness of the inverse problem is illustrated in [Kre19] by means of a simple example in which the solution v^i to the Helmholtz equation, given by $v^i(x) = \sin(k|x|)/|x|$, $x \in \mathbb{R}^3$, was considered as an incident field.

In this thesis, we only address the inverse shape reconstruction problem, whereas it is also possible to consider the more general inverse shape and impedance problem for identifying $\partial D, \mu$ and λ, see, e.g., [KR01, HKS09, CKS10, BCH12, CHK14, KR18] or the inverse impedance problem for determining the impedance functions for a known shape D, see, e.g., [Kre18, Yam19, YL21, YÖ25].

4.1. The Inverse Shape Problem

Due to Sommerfeld's radiation condition (2.6), the scattered wave has the asymptotic behavior

$$u^s(x) = \frac{\mathrm{e}^{\mathrm{i}k|x|}}{|x|^{\frac{d-1}{2}}} \left(u_\infty(\hat{x}) + \mathcal{O}\left(\frac{1}{|x|}\right)\right) \quad \text{for} \quad |x| \to \infty,$$

uniformly in all directions $\hat{x} = x/|x|$. The function u_∞ defined on the unit sphere S^{d-1} is called the far-field pattern of u^s. The behavior of the fundamental solution Φ of the Helmholtz equation and Green's representation theorem leads to the following description of the far-field pattern

$$u_\infty(\hat{x}) = \gamma_d \int_{\partial D} \left(u(y) \frac{\partial \mathrm{e}^{-\mathrm{i}k\hat{x}\cdot y}}{\partial \nu} - \frac{\partial u(y)}{\partial \nu} \mathrm{e}^{-\mathrm{i}k\hat{x}\cdot y} \right) \mathrm{d}s_y \,, \quad \widehat{x} \in S^{d-1}, \tag{4.1}$$

with $\gamma_2 = \mathrm{e}^{\mathrm{i}\pi/4}/\sqrt{8\pi k}$ and $\gamma_3 = 1/(4\pi)$, respectively, see [Het98b].

For a fixed incident field u^i, the solution to the direct scattering problem defines the domain-to-far-field operator $F\colon \partial D \mapsto u_\infty$, which maps the boundary ∂D of the scattering object onto the far-field pattern u_∞ of the scattered wave u^s. The inverse problem at hand consists of identifying D based on the known far-field pattern u_∞ and is expressed by the operator equation

$$F(\partial D) = u_\infty, \tag{4.2}$$

where F maps a class of admissible boundaries onto $L^2(S^{d-1})$. The direct scattering problem is nonlinear and well-posed, as we have seen in Chapter 2, while the operator equation (4.2), i.e., the inverse scattering problem, is nonlinear and ill-posed, see, e.g., [Kre18, Kre19]. The nonlinearity stems from the fact that the solution to the direct problem is nonlinear with respect to the boundary. Due to the analytical nature of the far-field pattern, the far-field mapping is extremely smoothing, which means that the solution of the nonlinear operator equation (4.2) is expected to be ill-posed in the sense of Hadamard, see [CK18].

Normally, the far-field data u_∞ is only known from noisy measurements, i.e., only the perturbed data u_∞^δ are given that fulfill

$$\|u_\infty^\delta - u_\infty\|_{L^2(S^{d-1})} \le \delta.$$

Discretization and numerical errors add further disturbances to the data, so no reliable results can be expected without using a regularization method.

To reconstruct the shape of the scattering object, iterative methods such as regularized Newton methods or nonlinear Landweber iterations can be used. In this thesis, we focus on a Newton-type method and analyze its performance. For this purpose, the existence and representation of the derivative of the domain-to-far-field operator F is important. In Section 3.2, we have derived a representation of the domain derivative, which we can then use to characterize F'. We have shown that F is differentiable in the sense that

$$\lim_{\|h\|_{C^1}\to 0} \frac{1}{\|h\|_{C^1}} \|F(\partial D_h) - F(\partial D) - u'_\infty\|_{L^2(S^{d-1})} = 0,$$

where u'_∞ denotes the far-field pattern of the domain derivative u' with respect to the perturbation $h \in C_c^1(B_R)$.

The uniqueness of the inverse problem, which corresponds to the injectivity of the operator F, is an open problem in the case of linear generalized impedance boundary conditions with far-field patterns for a finite number of incident waves with different incident directions, as mentioned in [CK12]. For the inverse impedance problem in the linear case, uniqueness results were obtained under certain assumptions on λ and μ, see [BH10]. Also in the linear case, it was shown in [Kre18] that both the shape and the impedance functions of a scattering obstacle with generalized impedance conditions are uniquely determined by the far-field patterns for an infinite number of incident waves with different incident directions. This result cannot be easily extended to the nonlinear case, since the proof given in [Kre18] relies on the mixed reciprocity principle ([CK13, Thm. 3.16, Thm. 3.17]). However, the nonlinearity breaks the reciprocity. Therefore, in the nonlinear case, the uniqueness of the inverse shape problem remains an open question.

4.1.1. Starlike Domains

To define the operator F properly, we restrict ourselves to boundaries ∂D that can be parameterized by mapping them globally onto the unit sphere. More precisely, for the numerical study of the scattering problem, we consider only admissible domains in $\mathbb{R}^2$ that are starlike with respect to the origin.

Definition 4.1. A bounded domain $D \subseteq \mathbb{R}^2$ is called starlike with respect to the origin if there exists a 2π-periodic positive function $r \in C(0, 2\pi)$ such that

$$\partial D = \{x(t) = r(t)(\cos t, \sin t)^\top : t \in [0, 2\pi]\}.$$

Hereinafter, we denote the far-field map F by $F\colon r \mapsto u_\infty$, where r belongs to the set $\{r \in C_p^2(0, 2\pi) : r > 0\}$ and indicates the radial component of the starlike boundary. This means that the operator F has a Fréchet derivative given by $F'[\partial D]h = u'_\infty$ for every admissible boundary ∂D and perturbation $h \in C_c^1(B_R)$. The parameterization of the update ∂D_{x+h} is not unique. The simplest way to avoid this ambiguity is to allow only perturbations of the form

$$h(x(t)) = \widetilde{h}(t)(\cos(t), \sin(t))^\top, \quad t \in [0, 2\pi],$$

with a scalar function $\widetilde{h}$, see [CK18].

4.2. Solution of the Inverse Problem

We suggest an all-at-once Newton-type method based on linearization of the forward problem and the domain-to-far-field operator. More precisely, at each iteration step, we update the solution by considering the $\mathbb{R}$-linear scattering problem and solving the linearized and regularized operator equation associated with (4.2). All-at-once methods have been used in various contexts, see for example [SHC98, HA01, HAO04, Kal16, Kal17, Rie21]. A comparison of the presented method with existing research can be found in section 4.7.

We begin by solving the linearized forward problem iteratively, replacing u by $u_n = u^i + u_n^s$ in each iteration step. Choosing initial guesses ∂D_0 and u_{-1}, we compute the solution u_n of the Helmholtz equation

$$\Delta u_n + k^2 u_n = 0 \quad \text{in } \Omega_{R,n} := B_R \backslash \overline{D_n}\,, \tag{4.3}$$

satisfying the boundary condition

$$\frac{\partial u_n}{\partial \nu} + \mathrm{i}k\Big(\lambda u_n - \mathrm{Div}(\mu \nabla_\tau u_n)\Big) - g_z(\cdot, u_{n-1}; u_n) = g(\cdot, u_{n-1}) - g_z(\cdot, u_{n-1}; u_{n-1}) \tag{4.4}$$

on ∂D_n. In addition, the scattered wave $u_n^s = u_n - u^i$ fulfills the Sommerfeld radiation condition (2.6). Note that the boundary condition is obtained by linearizing the nonlinear term $g(\cdot, u_n)$ in the sense of (3.10), i.e.,

$$g(\cdot, u_n) - g(\cdot, u_{n-1}) \approx \; g_z(\cdot, u_{n-1}; u_n - u_{n-1}).$$

Here, the previous iteration u_{n-1} is projected onto D_n, i.e., $u_{n-1}(r_n) = u_{n-1}(\mathcal{P}(r_{n-1}))$, where $\mathcal{P}$

is the unique projection of r_{n-1} onto ∂D_n.

It is known that boundary integral equations solved by Nyström's method are suitable for solving the scattering problem (4.3)–(4.4). Therefore, we consider a single-layer potential ansatz

$$u_n^s(x) = \mathrm{SL}\varphi_n(x) = \int_{\partial D_n} \Phi(x,y)\varphi_n(y)\,\mathrm{d}s_y \quad \text{for } x \in \Omega_{R,n} \tag{4.5}$$

for the scattered wave with a density $\varphi_n \in C(\partial D_n)$ and the fundamental solution Φ of the Helmholtz equation. Using the jump relations (2.24) and (2.25) for the single-layer potential, the scattered wave $u_n^s = u_n - u^i$ defined by (4.5) is a radiating solution of the Helmholtz equation, satisfying the impedance boundary condition (4.4) on ∂D_n if and only if the density φ_n solves the integral equation

$$-\frac{1}{2}\varphi_n + \mathcal{D}'\varphi_n + \mathrm{i}k\Big(\lambda\mathcal{S}\varphi_n - \mathrm{Div}(\mu\nabla_\tau\mathcal{S}\varphi_n)\Big) - g_z(\cdot, u_{n-1}; \mathcal{S}\varphi_n) = f \tag{4.6}$$

with

$$f = -\frac{\partial u^i}{\partial\nu} - \mathrm{i}k\Big(\lambda u^i - \mathrm{Div}(\mu\nabla_\tau u^i)\Big) + g(\cdot, u_{n-1}) + g_z(\cdot, u_{n-1}; u^i) - g_z(\cdot, u_{n-1}; u_{n-1}).$$

After presenting an approach to solving the direct problem by linearizing the boundary condition, we now address the nonlinear operator equation (4.2). Here, linearization leads to

$$F(r) + F'[r]h = u_\infty, \tag{4.7}$$

whereby we can improve the approximate boundary curve given by the radial function r to a new approximation $r + h$. The Newton method consists of solving equation (4.7) iteratively, i.e., replacing r by $r_{n+1} = r_n + h_n$, which results in

$$F_n(r_n) + F_n'[r_n]h_n = u_\infty^\delta\,. \tag{4.8}$$

Since the far-field data u_∞ is only known from imprecise data, we use u_∞^δ with an error level $\delta > 0$ on the right-hand side. Using the far-field pattern (4.1), the far-field $F_n(r_n) = u_{n,\infty}$ can be evaluated in each step. The Fréchet derivative of F_n is given by $F_n'[r_n]h_n = u_{n,\infty}'$, which corresponds to the far-field pattern of the domain derivative. For the iterative calculation, we replace u on the right-hand side of the boundary condition (3.17) by u_n.

Since the ill-posed linear operator equation (4.8) requires a regularization, we apply, as for the regularized Levenberg-Marquardt method, a Tikhonov regularization in any iteration step, which finally leads to the update h_n, given as the solution of

$$\big((F_n'[r_n])^* F_n'[r_n] + \alpha I\big)h_n = (F_n'[r_n])^*\big(u_\infty^\delta - F_n(r_n)\big), \tag{4.9}$$

where $\alpha > 0$ denotes a positive regularization parameter, see [Han97].

For such an iterative regularization method, a stopping rule is required, because the approximations will deteriorate for noisy data after a certain number of iterations. The most commonly used stopping rule is the discrepancy principle, where the method is terminated after the first iteration n for which it holds that

$$\|F_n(r_n) - u_\infty^\delta\|_{L^2(S^1)} \leq \tau\delta \quad \text{for some } \tau > 1, \tag{4.10}$$

i.e., as soon as the discrepancy between the computed far-field after the n-th step and the measured data has fallen below a certain threshold, see, e.g., [Kre03].

In summary, the integral equation constrained minimization problem, which fully captures the inverse problem under consideration, has the following form

$$\begin{aligned} &\min \quad \|F_n(r_n) + F_n'[r_n]h_n - u_\infty^\delta\|_{L^2(S^1)}^2 + \alpha\|h_n\|_{L^2(S^1)}^2 \\ &\text{s.t.} \quad -\frac{1}{2}\varphi_n + \mathcal{D}'\varphi_n + \mathrm{i}k\Big(\lambda\mathcal{S}\varphi_n - \mathrm{Div}(\mu\nabla_\tau\mathcal{S}\varphi_n)\Big) - g_z(\cdot, u_{n-1}; \mathcal{S}\varphi_n) - f = 0 \quad \text{on } \partial D_n. \end{aligned}$$

This formulation has the advantage that only the $\mathbb{R}$-linear model appears in the constraint, and we therefore do not need to invert the Nemystkii operator G with $G(\mathcal{S}\varphi_n)(\cdot) = g(\cdot, \mathcal{S}\varphi_n)$ for the calculation of φ_n.

Since we only solve the forward problem and the operator equation associated with the inverse problem approximately, the question of the convergence of the presented method arises.

4.2.1. Convergence

Convergence of the direct problem.

The linearization of nonlinear operators and the convergence of approximate solutions were investigated for various problems. For example, the convergence of the approximate solution to a nonlinear Sturm-Liouville type problem was proven in [Has00]. Here, Hasanov used a convexity argument as a sufficient condition for the convergence of the abstract iteration scheme for monotone potential operators. These results were subsequently extended in [Has04].

At present, we can only conjecture the convergence of the solution of the linearized problem ($\mathrm{SP}_{\mathrm{lin}}$) to the solution of the nonlinear problem (SP) based on numerical examples. A convergence study for the scattering problem presented in this thesis could be the subject of future investigations.

Convergence of the inverse problem.

The convergence of regularized Newton iterations for the operator F has not yet been clarified. It remains unclear whether the convergence results for the Levenberg-Marquardt algorithm obtained in recent decades are applicable to inverse obstacle scattering. This is mainly because the available convergence results always require a tangential cone condition for the nonlinearity of the form

$$\|F(r) - F(\hat{r}) - F'[r](r - \hat{r})\|_{L^2(S^1)} \leq c\|r - \hat{r}\|_{L^2(S^1)}\|F(r) - F(\hat{r})\|_{L^2(S^1)} \tag{4.11}$$

locally in a neighborhood of the exact solution in suitable Hilbert spaces, which, however, could not be confirmed for inverse obstacle scattering problems so far, see [Kre03]. Promising attempts to clarify the convergence of Newton iterations for inverse obstacle problems within the theoretical framework of nonlinear operator equations can be found in [Hoh97, Hoh98, Hoh99]. Convergence results for all-at-once versions of Newton-type regularization methods, under certain structural assumptions, were shown in [KKV14, Kal16, Kal17].

Even though we cannot make a convergence statement without assuming condition (4.11) it is known that, with a suitable choice of the regularization parameter in the regularized Levenberg-Marquardt method, very accurate reconstructions of the unknown scatterer from the far-field pattern can be achieved for one (or multiple) incident plane waves, as we will demonstrate in Chapter 5.

Before we examine the numerical performance of the presented all-at-once Newton-type method, we will take a closer look at the discrete schemes used to solve the direct and inverse problems in the following sections of this chapter. We begin with the Nyström method, which is well suited for solving the integral equation (4.6).

4.3. Nyström Method

In this section, we outline the Nyström method, which is a highly efficient method for approximating solutions to second-order boundary integral equations with continuous or weakly singular kernels, see, e.g., [Kre14, Sec. 12.2], [CK13, Sec. 3.5]. The method consists of approximating the integrals in a straightforward manner using quadrature formulas.

We assume that the boundary curve ∂D is given by a 2π-periodic parameterization

$$\partial D = \{\gamma(t) : t \in [0, 2\pi]\},$$

and introduce for $s \in [-1, 1]$ the parameterized operators

$$\widetilde{\mathcal{S}} \colon H_{\mathrm{per}}^{-\frac{1}{2}+s}[0, 2\pi] \to H_{\mathrm{per}}^{\frac{1}{2}+s}[0, 2\pi] \quad \text{and} \quad \widetilde{\mathcal{D}}' \colon H_{\mathrm{per}}^{-\frac{1}{2}+s}[0, 2\pi] \to H_{\mathrm{per}}^{-\frac{1}{2}+s}[0, 2\pi]$$

defined by

$$\begin{aligned}
\widetilde{\mathcal{S}}\psi(t) &:= \frac{\mathrm{i}}{4} \int_0^{2\pi} H_0^{(1)}(k|\gamma(t) - \gamma(\tau)|)|\gamma'(\tau)|\psi(\tau)\,\mathrm{d}\tau\,, \\
\widetilde{\mathcal{D}}'\psi(t) &:= \frac{\mathrm{i}k}{4} \int_0^{2\pi} \frac{[\gamma'(t)]^{\perp} \cdot [\gamma(\tau) - \gamma(t)]}{|\gamma'(t)||\gamma(t) - \gamma(\tau)|} H_1^{(1)}(k|\gamma(t) - \gamma(\tau)|)|\gamma'(\tau)|\psi(\tau)\,\mathrm{d}\tau\,,
\end{aligned}$$

for $t \in [0, 2\pi]$, see [Kre18]. Note that $H_0^{(1)}$ and $H_1^{(1)}$ denote the Hankel function of the first kind of order zero and one, respectively.

The second-order differential operator $\mathrm{Div}(\mu\nabla_\tau\cdot)$, which appears in the integral equation due to the use of a generalized impedance boundary condition, reduces in the two-dimensional case to

$$\varphi \mapsto \frac{\mathrm{d}}{\mathrm{d}s}\mu\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{S}\varphi.$$

Accordingly, the integral equation (4.6) in parameterized form is given by

$$-\frac{1}{2}\psi_n + \widetilde{\mathcal{D}}'\psi_n + \mathrm{i}k(\lambda \circ \gamma)\widetilde{\mathcal{S}}\psi_n - \mathrm{i}k\frac{1}{|\gamma'|}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mu \circ \gamma}{|\gamma'|}\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\mathcal{S}}\psi_n\right) - g_z(\cdot, u_{n-1}; \widetilde{\mathcal{S}}\psi_n) = f \circ \gamma.$$

In the following, we denote the kernel function of the parameterized single-layer operator $\widetilde{\mathcal{S}}$ by $M(t,s)$ and the one of the parameterized adjoint double-layer operator $\widetilde{\mathcal{D}}'$ by $L(t,s)$. For an appropriate numerical treatment, we decompose the kernels in accordance with Martensen ([Mar63]) and Kussmaul ([Kus69]) into

$$\begin{aligned} M(t,s) &= M_1(t,s)\ln\left(4\sin^2\frac{t-s}{2}\right) + M_2(t,s),\\ L(t,s) &= L_1(t,s)\ln\left(4\sin^2\frac{t-s}{2}\right) + L_2(t,s), \end{aligned}$$

where M_1, M_2, L_1 and L_2 are analytical functions.

As mentioned, the Nyström method consists of approximating the integrals by quadrature formulas. To approximate $\widetilde{\mathcal{S}}$ by $\widetilde{\mathcal{S}}_n$, we choose $2n$ equidistant nodal points $t_j = (\pi j)/n$, $j = 1, \dots, 2n$, and use the trapezoidal rule for the smooth part, i.e.,

$$\int_0^{2\pi} M_2(t,\tau)\psi_n(\tau)\,\mathrm{d}\tau \;\approx\; \frac{\pi}{n}\sum_{j=1}^{2n} M_2(t,t_j)\psi_n(t_j),$$

while the quadrature rule is applied to the weakly singular residual

$$\int_0^{2\pi} M_1(t,\tau)\ln\left(4\sin^2\frac{t-\tau}{2}\right)\psi_n(\tau)\,\mathrm{d}\tau \;\approx\; \sum_{j=1}^{2n} R_j^{(n)}(t) M_1(t,t_j)\psi_n(t_j), \quad 0 \le t \le 2\pi,$$

with the quadrature weights given by

$$R_j^{(n)}(t) = -\frac{2\pi}{n}\sum_{m=1}^{n-1}\frac{1}{m}\cos(m(t-t_j)) - \frac{\pi}{n^2}\cos(n(t-t_j)) \quad \text{for } j = 0, \dots, 2n-1.$$

Analogously, the approximation $\widetilde{\mathcal{D}}'_n$ can be obtained by replacing M_1 and M_2 by L_1 and L_2 respectively. For more details, see [CK13, Sec. 3.5]. Lastly, we need an approximation for the operator

$$\psi \mapsto \frac{1}{|\gamma'|}\frac{\mathrm{d}}{\mathrm{d}t}\frac{(\mu\circ\gamma)}{|\gamma'|}\frac{\mathrm{d}}{\mathrm{d}t}\psi\,,$$

for which we use trigonometric differentiation as suggested in the works [CK12] and [Kre18]. The idea is to utilize a trigonometric polynomial $P_n\psi$ that interpolates the function ψ at the nodal points t_j. Then the derivative $(P_n\psi)'$ can be used as an approximation of the derivative ψ'. Specifically, the derivative of the trigonometric polynomial is given by

$$P_n'\psi(t_j) := (P_n\psi)'(t_j) = \sum_{k=1}^{2n} d_{|k-j|}^{(n)}\psi(t_k) \quad \text{for } j = 1, \dots, 2n,$$

with weights

$$d_j = \begin{cases} \frac{(-1)^j}{2}\cot\left(\frac{j\pi}{2n}\right), & j = 1, \dots, 2n-1,\\ 0, & j = 0. \end{cases}$$

Taking the above considerations into account, a suitable finite-dimensional approximation of the integral equation (4.6) can be formulated. For the sake of simplicity, we introduce the functions

$$\widetilde{M}(t,t_j) := R_j^{(n)}(t)M_1(t,t_j) + \frac{\pi}{n}M_2(t,t_j),$$
$$\widetilde{L}(t,t_j) := R_j^{(n)}(t)L_1(t,t_j) + \frac{\pi}{n}L_2(t,t_j),$$

for $j = 1,\dots,2n$. Therefore, in the discrete setting, the function ψ_n is a solution of the $\mathbb{R}$-linear system

$$\begin{aligned}
&-\frac{1}{2}\psi_n(t) + \sum_{j=1}^{2n}\widetilde{L}(t,t_j)\psi_n(t) + \mathrm{i}k(\lambda\circ\gamma)(t)\sum_{j=1}^{2n}\widetilde{M}(t,t_j)\psi_n(t_j)\\
&-\mathrm{i}k\frac{1}{|\gamma'(t)|}P_n'\frac{(\mu\circ\gamma)(t)}{|\gamma'(t)|}P_n'\sum_{j=1}^{2n}\widetilde{M}(t,t_j)\psi_n(t_j) + g_z\left(\cdot,u_{n-1};\sum_{j=1}^{2n}\widetilde{M}(t,t_j)\psi_n(t_j)\right)\\
&=(f\circ\gamma)(t),
\end{aligned}$$

for $t\in[0,2\pi]$. In the following, we use an abbreviated notation of the equation, which is depicted by

$$-\frac{1}{2}\psi_n + \widetilde{\mathcal{D}}_n'\psi_n + \mathrm{i}k(\lambda\circ\gamma)\widetilde{\mathcal{S}}_n\psi_n - \mathrm{i}k\frac{1}{|\gamma'|}P_n'\frac{(\mu\circ\gamma)}{|\gamma'|}P_n'\widetilde{\mathcal{S}}_n\psi_n - g_z(\cdot,u_{n-1};\widetilde{\mathcal{S}}_n\psi_n) = f\circ\gamma. \quad (4.12)$$

One question that remains is how we deal with the $\mathbb{R}$-linear term $g_z(\cdot,u_{n-1};\widetilde{\mathcal{S}}_n\psi_n)$, because if $\widetilde{\mathcal{S}}_n\psi_n$ contains complex entries, it is not guaranteed that we can write $\widetilde{\mathcal{S}}_n\psi_n$ outside the brackets. For example, if we consider the cubic Kerr nonlinearity $g(\cdot,u) = |u|^2u$, then

$$g_z(\cdot,u;z) = |u|^2 + 2\mathrm{Re}\,(\overline{u}z)u \begin{cases} = g_z(\cdot,u;1)z, & \text{for } z\in\mathbb{R}, \text{ but}\\ \neq g_z(\cdot,u;1)z, & \text{for } z\in\mathbb{C}.\end{cases}$$

Depending on which nonlinearity is considered, the numerical calculation of the solution ψ_n of (4.12) can be challenging. To circumvent this difficulty, we follow the idea from Section 2.4 by decomposing $\widetilde{\mathcal{S}}_n\psi_n$ into its real and imaginary parts.

We consider the boundary integral equation (4.12) with the $\mathbb{R}$-linear operator

$$\mathcal{A}\psi_n = -\frac{1}{2}\psi_n + \widetilde{\mathcal{D}}_n'\psi_n + \mathrm{i}k(\lambda\circ\gamma)\widetilde{\mathcal{S}}_n\psi_n - \mathrm{i}k\frac{1}{|\gamma'|}P_n'\frac{(\mu\circ\gamma)}{|\gamma'|}P_n'\widetilde{\mathcal{S}}_n\psi_n - g_z(\cdot,u_{n-1};\widetilde{\mathcal{S}}_n\psi_n)$$

and right-hand side $f\circ\gamma$. In order to find a real matrix representation for the operator $\mathcal{A}$ as in (2.33), we require the $\mathbb{R}$-linear term $g_z(\cdot,u_{n-1};\widetilde{\mathcal{S}}_n\psi_n)$ to admit a representation of the form

$$g_z(\cdot,u_{n-1};\widetilde{\mathcal{S}}_n\psi_n) = g_z(\cdot,u_{n-1};\mathbb{1})\mathrm{Re}\,(\widetilde{\mathcal{S}}_n\psi_n) + \mathrm{i}g_z(\cdot,\xi u_{n-1};\mathbb{1})\mathrm{Im}\,(\widetilde{\mathcal{S}}_n\psi_n) \quad (4.13)$$

for a $\xi\in\mathbb{C}$, depending on the chosen nonlinearity. In this context, $\mathbb{1}$ denotes the vector of ones of appropriate size. For such a decomposition in the case of cubic Kerr nonlinearity, as well as for the nonlinearity from Remark 2.8 (i), see Example 4.2 below. This allows us to specify the entries of the real matrix

$$\phi(\mathcal{A}) = \begin{bmatrix} \mathrm{Re}(A + A_{\#}) & \mathrm{Im}(-A + A_{\#}) \\ \mathrm{Im}(A + A_{\#}) & \mathrm{Re}(A - A_{\#}) \end{bmatrix},$$

which are given by

$$\begin{aligned}
\mathrm{Re}\,(A + A_{\#}) = &- \frac{1}{2}I + \mathrm{Re}\,(\widetilde{\mathcal{D}}'_n) - k\mathrm{Re}\,(\lambda \circ \gamma)\mathrm{Im}\,(\widetilde{\mathcal{S}}_n) - k\mathrm{Im}\,(\lambda \circ \gamma)\mathrm{Re}\,(\widetilde{\mathcal{S}}_n) \\
&+ \frac{k}{|\gamma'|}P'_n \frac{\mathrm{Re}\,(\mu \circ \gamma)}{|\gamma'|}P'_n \mathrm{Im}\,(\widetilde{\mathcal{S}}_n) + \frac{k}{|\gamma'|}P'_n \frac{\mathrm{Im}\,(\mu \circ \gamma)}{|\gamma'|}P'_n \mathrm{Re}\,(\widetilde{\mathcal{S}}_n) \\
&- \mathrm{Re}\,(g_z(\cdot, u_{n-1}; \mathbb{1}))\mathrm{Re}\,(\widetilde{\mathcal{S}}_n) + \mathrm{Im}\,(g_z(\cdot, \xi u_{n-1}; \mathbb{1}))\mathrm{Im}\,(\widetilde{\mathcal{S}}_n),
\end{aligned}$$

$$\begin{aligned}
\mathrm{Im}\,(-A + A_{\#}) = &- \mathrm{Im}\,(\widetilde{\mathcal{D}}'_n) - k\mathrm{Re}\,(\lambda \circ \gamma)\mathrm{Re}\,(\widetilde{\mathcal{S}}_n) + k\mathrm{Im}\,(\lambda \circ \gamma)\mathrm{Im}\,(\widetilde{\mathcal{S}}_n) \\
&+ \frac{k}{|\gamma'|}P'_n \frac{\mathrm{Re}\,(\mu \circ \gamma)}{|\gamma'|}P'_n \mathrm{Re}\,(\widetilde{\mathcal{S}}_n) - \frac{k}{|\gamma'|}P'_n \frac{\mathrm{Im}\,(\mu \circ \gamma)}{|\gamma'|}P'_n \mathrm{Im}\,(\widetilde{\mathcal{S}}_n) \\
&+ \mathrm{Re}\,(g_z(\cdot, u_{n-1}; \mathbb{1}))\mathrm{Im}\,(\widetilde{\mathcal{S}}_n) + \mathrm{Im}\,(g_z(\cdot, \xi u_{n-1}; \mathbb{1}))\mathrm{Re}\,(\widetilde{\mathcal{S}}_n),
\end{aligned}$$

$$\begin{aligned}
\mathrm{Im}\,(A + A_{\#}) = &\ \mathrm{Im}\,(\widetilde{\mathcal{D}}'_n) + k\mathrm{Re}\,(\lambda \circ \gamma)\mathrm{Re}\,(\widetilde{\mathcal{S}}_n) - k\mathrm{Im}\,(\lambda \circ \gamma)\mathrm{Im}\,(\widetilde{\mathcal{S}}_n) \\
&- \frac{k}{|\gamma'|}P'_n \frac{\mathrm{Re}\,(\mu \circ \gamma)}{|\gamma'|}P'_n \mathrm{Re}\,(\widetilde{\mathcal{S}}_n) + \frac{k}{|\gamma'|}P'_n \frac{\mathrm{Im}\,(\mu \circ \gamma)}{|\gamma'|}P'_n \mathrm{Im}\,(\widetilde{\mathcal{S}}_n) \\
&- \mathrm{Im}\,(g_z(\cdot, u_{n-1}; \mathbb{1}))\mathrm{Re}\,(\widetilde{\mathcal{S}}_n) - \mathrm{Re}\,(g_z(\cdot, \xi u_{n-1}; \mathbb{1}))\mathrm{Im}\,(\widetilde{\mathcal{S}}_n),
\end{aligned}$$

$$\begin{aligned}
\mathrm{Re}\,(A - A_{\#}) = &- \frac{1}{2}I + \mathrm{Re}\,(\widetilde{\mathcal{D}}'_n) - k\mathrm{Re}\,(\lambda \circ \gamma)\mathrm{Im}\,(\widetilde{\mathcal{S}}_n) - k\mathrm{Im}\,(\lambda \circ \gamma)\mathrm{Re}\,(\widetilde{\mathcal{S}}_n) \\
&+ \frac{k}{|\gamma'|}P'_n \frac{\mathrm{Re}\,(\mu \circ \gamma)}{|\gamma'|}P'_n \mathrm{Im}\,(\widetilde{\mathcal{S}}_n) + \frac{k}{|\gamma'|}P'_n \frac{\mathrm{Im}\,(\mu \circ \gamma)}{|\gamma'|}P'_n \mathrm{Re}\,(\widetilde{\mathcal{S}}_n) \\
&+ \mathrm{Im}\,(g_z(\cdot, u_{n-1}; \mathbb{1}))\mathrm{Im}\,(\widetilde{\mathcal{S}}_n) - \mathrm{Re}\,(g_z(\cdot, \xi u_{n-1}; \mathbb{1}))\mathrm{Re}\,(\widetilde{\mathcal{S}}_n).
\end{aligned}$$

By inverting the matrix $\phi(\mathcal{A})$, the real and imaginary parts of the function ψ_n that solves the integral equation (4.12) can be calculated, i.e.,

$$\begin{pmatrix} \mathrm{Re}\,(\psi_n) \\ \mathrm{Im}\,(\psi_n) \end{pmatrix} = (\phi(\mathcal{A}))^{-1} \begin{pmatrix} \mathrm{Re}\,(f \circ \gamma) \\ \mathrm{Im}\,(f \circ \gamma) \end{pmatrix}.$$

Using the example of a cubic Kerr nonlinearity or the function g from Remark 2.8 (i), a division of g_z in the sense of (4.13) can easily be found.

Example 4.2. (i) The linearization of the Kerr-type nonlinearity $g(\cdot, u) = |u|^2 u$ is given by

$$g_z(\cdot, u; z) = |u|^2 z + 2\mathrm{Re}\,(\overline{u}z)u.$$

Splitting z into its real and imaginary parts provides

$$\begin{aligned}
g_z(\cdot, u; z) &= |u|^2 \left(\mathrm{Re}\,(z) + \mathrm{i}\mathrm{Im}\,(z)\right) + 2\left(\mathrm{Re}\,(\overline{u})\mathrm{Re}\,(z) + \mathrm{Im}\,(-\overline{u})\mathrm{Im}\,(z)\right) u \\
&= \left(|u|^2 + 2\mathrm{Re}\,(\overline{u})u\right) \mathrm{Re}\,(z) + \left(\mathrm{i}|u|^2 + 2\mathrm{Im}\,(-\overline{u})u\right) \mathrm{Im}\,(z)
\end{aligned}$$

$$
\begin{aligned}
&= g_z(\cdot, u; \mathbb{1})\mathrm{Re}\,(z) + \mathrm{i}\left(|u|^2 + 2\mathrm{Re}\,(\overline{-\mathrm{i}u})(-\mathrm{i}u)\right)\mathrm{Im}\,(z) \\
&= g_z(\cdot, u; \mathbb{1})\mathrm{Re}\,(z) + \mathrm{i}g_z(\cdot, -\mathrm{i}u; \mathbb{1})\mathrm{Im}\,(z).
\end{aligned}
$$

Therefore, we obtain the required decomposition (4.13) of g_z with $\xi = -\mathrm{i}$.

(ii) For the nonlinear function $g(\cdot, u) = u/(1 + |u|^2)$, the linearization is given by

$$
g_z(\cdot, u; z) = \frac{(1 + |u|^2)z - 2\mathrm{Re}\,(\overline{u}z)u}{(1 + |u|^2)^2}\,,
$$

as we have seen in Example 2.10 (ii). With a similar calculation as in (i), we obtain

$$
\begin{aligned}
g_z(\cdot, u; z) &= \frac{(1 + |u|^2)\left(\mathrm{Re}\,(z) + \mathrm{i}\mathrm{Im}\,(z)\right)}{(1 + |u|^2)^2} - \frac{2\left(\mathrm{Re}\,(\overline{u})\mathrm{Re}\,(z) + \mathrm{Im}\,(-\overline{u})\mathrm{Im}\,(z)\right)u}{(1 + |u|^2)^2} \\
&= \frac{1 + |u|^2 - 2\mathrm{Re}\,(\overline{u})u}{(1 + |u|^2)^2}\,\mathrm{Re}\,(z) + \frac{\mathrm{i}(1 + |u|^2) - 2\mathrm{Im}\,(-\overline{u})u}{(1 + |u|^2)^2}\,\mathrm{Im}\,(z) \\
&= g_z(\cdot, u; \mathbb{1})\mathrm{Re}\,(z) + \frac{(1 + |u|^2) - 2\mathrm{Re}\,(\overline{\mathrm{i}u})(\mathrm{i}u)}{(1 + |u|^2)^2}\,\mathrm{i}\mathrm{Im}\,(z) \\
&= g_z(\cdot, u; \mathbb{1})\mathrm{Re}\,(z) + \mathrm{i}g_z(\cdot, \mathrm{i}u; \mathbb{1})\mathrm{Im}\,(z).
\end{aligned}
$$

For this nonlinearity, we must therefore choose $\xi = \mathrm{i}$ in (4.13). △

For the proposed Newton method (4.8), we need to evaluate the Fréchet derivative of the far-field operator F_n, which can be obtained from the far-field patterns of the domain derivative. Therefore, the next step is to solve the boundary value equation (3.16)–(3.18) for u_n'.

4.3.1. Discrete Domain Derivative

Since the domain derivative u_n' solves the Helmholtz equation in the exterior domain and a generalized impedance boundary condition on the boundary of the obstacle, we can use an equivalent integral equation formulation as in (4.12) to determine the solution of (3.16)–(3.18) numerically using Nyström's method. Note that, due to the right-hand side of the boundary condition (3.17), the Cauchy data

$$
u_n|_{\partial D_n} = \widetilde{\mathcal{S}}_n\psi_n + u^i \quad \text{and} \quad \frac{\partial u_n}{\partial \nu}\bigg|_{\partial D_n} = -\frac{1}{2}\psi_n + \widetilde{\mathcal{D}}_n'\psi_n + \frac{\partial u^i}{\partial \nu}
$$

are required for the computation of u_n', which we can specify using the solutions ψ_n from (4.12).

Hence, u_n' solves the scattering problem (3.16)–(3.18) if and only if $u_n'|_{\partial D}$ satisfies the boundary integral equation

$$
-\frac{1}{2}u_n' + \widetilde{\mathcal{D}}_n'u_n' + \mathrm{i}k(\lambda \circ \gamma)\widetilde{\mathcal{S}}_n u_n' - \mathrm{i}k\frac{1}{|\gamma'|}P_n'\frac{(\mu \circ \gamma)}{|\gamma'|}P_n'\widetilde{\mathcal{S}}_n u_n' - g_z(\cdot, u_{n-1}; \widetilde{\mathcal{S}}_n u_n') = \widehat{f} \circ \gamma, \quad (4.14)
$$

with the right-hand side

$$
\widehat{f} \circ \gamma = \frac{1}{|\gamma'|}P_n'\left(\frac{h_{\nu_n}}{|\gamma'|}P_n'u_n\right) + k^2 u_n h_{\nu_n} - \mathrm{i}k(\lambda \circ \gamma)\left(2\kappa_n u_n h_{\nu_n} + \frac{\partial u_n}{\partial \nu}h_{\nu_n}\right) - \mathrm{i}k\frac{\partial(\lambda \circ \gamma)}{\partial \nu}u_n h_{\nu_n}
$$

$$
+ \frac{\mathrm{i}k}{|\gamma'|} P_n' \left(h_{\nu_n} \left(2(\mu \circ \gamma)\kappa_n + \frac{\partial(\mu \circ \gamma)}{\partial \nu} - 2(\mu \circ \gamma) J_{\nu_n} \right) \frac{1}{|\gamma'|} P_n' u_n \right)
$$
$$
+ \frac{\mathrm{i}k}{|\gamma'|} P_n' \left(\frac{(\mu \circ \gamma)}{|\gamma'|} P_n' \left(\frac{\partial u_n}{\partial \nu} h_{\nu_n} \right) \right) + g_z \left(\cdot, u_n; \frac{\partial u_n}{\partial \nu} h_{\nu_n} \right) + 2\kappa_n g(\cdot, u_n) h_{\nu_n} \,.
$$

As shown in Section 3.2, the domain derivative u_n' depends only on the normal component h_{ν_n} of the perturbation on the boundary. Since we assume that the perturbation h_n is a 2π-periodic function approximated by trigonometric polynomials, the normal component of h_n is given by

$$
h_{\nu_n}(\gamma(t)) = h_n(\gamma(t)) \cdot \nu_n(\gamma(t)) = \frac{h_n(t) r_n(t)}{\sqrt{r_n'^2(t) + r_n^2(t)}}\,, \quad t \in [0, 2\pi].
$$

Furthermore, the curvature κ_n is defined by

$$
\kappa_n(t) = \frac{\det(\gamma_n'(t), \gamma_n''(t))}{|\gamma_n'(t)|^3} = \frac{2r_n'^2(t) - r_n(t) r_n''(t) + r_n^2(t)}{(r_n'^2(t) + r_n^2(t))^{3/2}}\,, \quad t \in [0, 2\pi],
$$

see, e.g., [Het98b].

With knowledge of the solution u_n to the direct scattering problem and the domain derivative u_n', we can now move on to the inverse problem, which we solve approximately using the linearized and regularized operator equation (4.9).

4.4. Regularized Newton Method

In equation (4.2), we introduced the far-field operator F as a mapping in $L^2(S^1)$. To calculate the update of the boundary curve using the regularized Newton method, we need both the Fréchet derivative F' of the far-field operator and its adjoint F'^*. A representation of these operators in the L^2 sense can be determined for the linear case, i.e., for $g \equiv 0$, by exploiting the reciprocity principle, see Appendix C. However, such a representation of the Fréchet derivative and its adjoint cannot be established for the nonlinear case, since we cannot assume, for example, that $g(\cdot, u)u'$ is equal to $g(\cdot, u')u$. We can circumvent this difficulty for the implementation of the algorithm by considering the derivative F' only in the discrete sense and thus also avoiding the calculation of the corresponding adjoint in $L^2(S^1)$.

The boundary variations are considered in the finite-dimensional subspace of trigonometric polynomials, i.e.,

$$
h(t) = \frac{1}{2} h_0 + \sum_{j=1}^{m} h_j^c \cos(jt) + h_j^s \sin(jt), \quad h_0, h_j^c, h_j^s \in \mathbb{R},\ j = 1, \ldots, m.
$$

Now $F'[r]$ operates on a finite set, and due to the linearity of $F'[r]$, we have

$$
F'[r]h = h_0 \left(\frac{1}{2} F'[r] \right) + \sum_{j=1}^{m} \left[h_j^{(c)} \left(F'[r] \cos(j\cdot) \right) + h_j^{(s)} \left(F'[r] \sin(j\cdot) \right) \right].
$$

By solving the integral equation (4.6) using the initial guess $u_0 = u^i$, the density φ_n can be determined for the approximate boundary curve ∂D_n. The far-field patterns $F_n(r_n) = u_{n,\infty}$ are then computed by

$$u_{n,\infty}(\hat{x}) = \frac{e^{\mathrm{i}\frac{\pi}{4}}}{\sqrt{8\pi k}} \int_{\partial D_n} e^{-\mathrm{i}k\hat{x}\cdot y} \varphi_n(y)\,\mathrm{d}s_y, \quad \hat{x} \in S^1. \tag{4.15}$$

Next, for each basis function $h(t) = \cos(jt)$ and $h(t) = \sin(jt)$, the domain derivative from Theorem 3.5 is obtained by solving the integral equation (4.14). Again using (4.15), we calculate the far-field patterns $F_n'[r_n]h = u_{n,\infty}'$ of the domain derivatives u_n' for all basis functions associated with the current boundary curve. Collecting these far-field patterns yields a Jacobian matrix $J \in \mathbb{R}^{(2n)\times(2m+1)}$ at the $2n$ nodal points chosen for the discretization, i.e.,

$$J := \left(\begin{array}{c|c|c} \frac{1}{2} F_n'[r_n] & F_n'[r_n]\cos(B) & F_n'[r_n]\sin(B) \end{array} \right), \quad \text{where} \;\; B = (b_{ij})_{\substack{i=1,\dots,2n,\\ j=1,\dots,m}} = jt_i\,.$$

Therefore, we obtain the following discrete equation

$$Jh_n = u_\infty^\delta - F_n(r_n),$$

where h_n contains the $2m + 1$ Fourier coefficients of h_n. The application of the Tikhonov regularization leads to

$$(J^*J + \alpha R)h_n = J^*(u_\infty^\delta - F_n(r_n))\,,$$

where we regularize with the diagonal matrix R, which approximates the effect of Tikhonov regularization with respect to the H^2-norm by penalizing higher Fourier modes more strongly. It is known that using an H^2-penalty that corresponds to the curvature of the boundary instead of an L^2-penalty improves the results for inverse acoustic scattering problems for star-shaped domains, see [Het99]. The entries of the diagonal matrix R are given by

$$R_{jj} = \begin{cases} 1 + j^2, & j = 0, \dots, n, \\ 1 + (j-n)^2, & j = n+1, \dots, 2n. \end{cases}$$

Typically, the iteration initially converges but diverges after a certain number of steps, see [Han97]. In order to obtain stable approximations of the boundary curve, a stopping rule must be specified. For the regularized Newton method presented here, it is known that the discrepancy principle provides a suitable stopping rule. Therefore, the iteration is stopped at index n for which

$$\|F_n(r_n) - u_\infty^\delta\|_2 \le \tau\delta, \quad \tau \in (1,2), \tag{4.16}$$

is valid for the first time. Here, the norm $\|\cdot\|_2$ denotes the Euclidean norm. For a broader overview of iterative regularization methods, we refer to [KNS08].

Next, we discuss which forward solver is used to generate the synthetic data u_∞^δ and to what extent it is independent of the inverse solver under consideration.

4.5. Inverse Crime

Since there are generally no explicit solutions known for the direct scattering problem, numerical evaluations of the inverse problem are usually based on the synthetic far-field data obtained by solving the forward scattering problem. To avoid trivial inversion of discrete problems, the synthetic data must be obtained by a forward solver that is independent of the considered inverse solver, see [CK13].

To avoid an inverse crime, we compute the synthetic data using a different integral equation approach for the scattered wave than in (4.5) and double the number of discretization points compared to the inverse solver. More precisely, in each iteration step, we consider the direct approach based on Green's representation theorem, from which we obtain the following representation

$$u_n^s(x) = \mathrm{DL}u_n(x) - \mathrm{SL}\frac{\partial u_n(x)}{\partial \nu} = \int_{\partial D} \frac{\partial \Phi(x,y)}{\partial \nu_y} u_n(y) - \Phi(x,y)\frac{\partial u_n(y)}{\partial \nu_y}\, \mathrm{d}s_y \quad \text{for } x \in \Omega_R.$$

The jump relations (2.24)–(2.26) of the single-layer and double-layer potential at the boundary ∂D_n and the linearized boundary condition (4.4) lead to the integral equation

$$\begin{aligned} \frac{1}{2}u_n - \mathcal{D}u_n - \mathcal{S}(\mathrm{i}k\lambda u_n) + \mathcal{S}(\mathrm{i}k\mathrm{Div}(\mu\nabla_\tau u_n)) + \mathcal{S}g_z(\cdot, u_{n-1}; u_n) \\ = u^i + \mathcal{S}\big(g_z(\cdot, u_{n-1}; u_{n-1}) - g(\cdot, u_{n-1})\big), \end{aligned} \tag{4.17}$$

where $\mathcal{D}$ denotes the boundary integral operator corresponding to the double-layer potential as defined in Definition 2.12.

Following Section 4.3, the integral equation (4.17) in discrete form is given by

$$\frac{1}{2}\widetilde{u}_n - \widetilde{\mathcal{D}}_n\widetilde{u}_n - \widetilde{\mathcal{S}}_n\mathrm{i}k(\lambda\circ\gamma)\widetilde{u}_n + \widetilde{\mathcal{S}}_n\mathrm{i}k\frac{1}{|\gamma'|}P_n'\frac{(\mu\circ\gamma)}{|\gamma'|}P_n'\widetilde{u}_n + \widetilde{\mathcal{S}}_n g_z(\cdot, \widetilde{u}_{n-1}; \widetilde{u}_n) = f\circ\gamma\,, \tag{4.18}$$

where $\widetilde{u}_n = u_n \circ \gamma$. For the operator

$$\mathcal{B}\widetilde{u}_n = \frac{1}{2}\widetilde{u}_n - \widetilde{\mathcal{D}}_n\widetilde{u}_n - \widetilde{\mathcal{S}}_n\mathrm{i}k(\lambda\circ\gamma)\widetilde{u}_n + \widetilde{\mathcal{S}}_n\mathrm{i}k\frac{1}{|\gamma'|}P_n'\frac{(\mu\circ\gamma)}{|\gamma'|}P_n'\widetilde{u}_n + \widetilde{\mathcal{S}}_n g_z(\cdot, \widetilde{u}_{n-1}; \widetilde{u}_n)\,,$$

we can again find a real-valued matrix representation $\phi(\mathcal{B})$ as described in Section 2.4.2, such that the real and imaginary part of the solution $\widetilde{u}_n$ to the integral equation (4.18) can be calculated by

$$\begin{pmatrix} \mathrm{Re}\,(\widetilde{u}_n) \\ \mathrm{Im}\,(\widetilde{u}_n) \end{pmatrix} = (\phi(\mathcal{B}))^{-1} \begin{pmatrix} \mathrm{Re}\,(f\circ\gamma) \\ \mathrm{Im}\,(f\circ\gamma) \end{pmatrix}.$$

The entries of the matrix $\phi(\mathcal{B})$ can be found in Appendix B.

Using the solution u_n of the integral equation (4.18), the synthetic far-field data can then be computed by

$$\widetilde{u}_{n,\infty}(\hat{x}) = -\frac{e^{\mathrm{i}\frac{\pi}{4}}}{\sqrt{8\pi k}} \int_{\partial D} \left(\mathrm{i}k(\nu_y\cdot\hat{x})\widetilde{u}_n(y) + \frac{\partial \widetilde{u}_n(y)}{\partial \nu}\right) e^{-\mathrm{i}k\hat{x}\cdot y}\, \mathrm{d}s_y\,, \quad \hat{x}\in S^1, \tag{4.19}$$

see [Het99].

To calculate the synthetic data, we perform $n = 10$ updates of the solution $\widetilde{u}_n$ to the scattering problem (4.18) and then calculate the corresponding far-field pattern of the approximate solution $\widetilde{u}_{10}$ using (4.19). In the numerical tests performed, we observed linear convergence, i.e.,

$\|\widetilde{u}_{n-1} - \widetilde{u}_n\|_{L^2} / \|\widetilde{u}_{n-2} - \widetilde{u}_{n-1}\|_{L^2} \leq p$ for $p \in (0, 1)$. In the examples considered in Chapter 5, machine precision is already achieved after $n = 5$ iteration steps for almost all shapes. Note that for the discrepancy principle (4.16) as a stopping condition, we only consider every second entry of the synthetic data $\widetilde{u}_{10,\infty}$ to ensure that the dimension matches that of $F_n(r_n)$.

4.6. Shape Reconstruction Algorithm

The pseudo code for the reconstruction of a two-dimensional scattering object, for which the superposition of the incident and the scattered wave satisfies the Helmholtz equation together with a nonlinear generalized impedance boundary condition on ∂D, is shown in Algorithm 1.

Algorithm 1 All-at-once regularized Newton method

Input: Initial guesses u_0 and r_0, wave number k, noise level δ.

Output: Approximation of forward problem and far-field pattern, update boundary curve.

1: Set $u_0 = u^i$, $r_0 =$ radius circle, $n = 0$.

2: Update $\varphi_n = \left(-\frac{1}{2}I + \mathcal{D}' + \mathrm{i}k\mathcal{S} - \mathrm{i}k\frac{\mathrm{d}}{\mathrm{d}s}\left(\mu\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{S}\cdot\right) - g_z(\cdot, u_n; \mathcal{S}\cdot)\right)^{-1} f$,

3: $u_{n+1} = \mathcal{S}\varphi_n + u^i$, $u_{n+1,\infty} = \mathrm{e}^{\mathrm{i}\pi/4}/\sqrt{8\pi k} \int_{\partial D_n} \mathrm{e}^{-\mathrm{i}ky\cdot}\varphi_n(y)\,\mathrm{d}s_y = F_n(r_n)$,

4: $\widetilde{\varphi}_n = \left(-\frac{1}{2}I + \mathcal{D}' + \mathrm{i}k\mathcal{S} - \mathrm{i}k\frac{\mathrm{d}}{\mathrm{d}s}\left(\mu\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{S}\cdot\right) - g_z(\cdot, u_{n+1}; \mathcal{S}\cdot)\right)^{-1} \widehat{f}(u_{n+1})$,

5: $u'_{n+1,\infty} = \mathrm{e}^{\mathrm{i}\pi/4}/\sqrt{8\pi k} \int_{\partial D_n} \mathrm{e}^{-\mathrm{i}ky\cdot}\widetilde{\varphi}_n(y)\,\mathrm{d}s_y = F'_n[r_n]h_n$,

6: $h_n = (F'_n[r_n]^* F'_n[r_n] + \alpha R)^{-1} \left[F'_n[r_n]^* \left(F_n(r_n) - u^\delta_\infty\right)\right]$,

7: $r_{n+1} = r_n + \mathrm{Re}\,(h_n)$,

8: $n = n + 1$.

9: **if** $\|F_n(r_n) - u^\delta_\infty\|_2 \leq \tau\delta$ **then**

10: Break.

11: **end if**

We call the shape reconstruction algorithm presented here an all-at-once method, since we update both the forward and inverse problems in each iteration step. However, the question arises to what extent this method is related to those described in the literature as all-at-once methods and what modifications we have made.

4.7. Modifications of the Reconstruction Method

Over the past few decades, the use of an all-at-once approach has become increasingly important, for example, in optimization under PDE constraints, see [SHC98, HA01, HAO04] and the references therein. In [HA01], for example, a preconditioned Krylov method was used to calculate the solution of the forward problem simultaneously with the solution of the inverse problem.

In the context of inverse and ill-posed problems, Kaltenbacher presented regularization results for abstract all-at-once formulations of Newton methods in [Kal16]. An extension of these results to time-dependent inverse problems can be found in [Kal17]. Furthermore, an all-at-once version of the full waveform seismic inversion was presented in [Rie21].

For parameter identification problems, as in the references mentioned above, the idea of an all-at-once method consists of determining a parameter p from observations of the state u, where the state u satisfies an equation model $A(p, u) = 0$.

A straightforward transfer of this formulation to the inverse scattering problem from Section 4.1 would be given by

$$\mathbb{F}(r, g) = \begin{pmatrix} A(r, g) \\ F(r) \end{pmatrix} = \begin{pmatrix} 0 \\ u_\infty^\delta \end{pmatrix}, \tag{4.20}$$

where F denotes the far-field operator defined in (4.2) and $A(r, g(\cdot, u)) = 0$ is an equation model for the state u that solves the direct scattering problem (SP). Linearization of (4.20) leads to

$$\mathbb{F}(r, g) + \mathbb{F}'[r, g] \begin{pmatrix} h \\ v \end{pmatrix} = \begin{pmatrix} A(r, g) \\ F(r) \end{pmatrix} + \begin{pmatrix} \partial_r A(r, g; h) + \partial_g A(r, g; v) \\ F'[r]h \end{pmatrix} \approx \begin{pmatrix} 0 \\ u_\infty^\delta \end{pmatrix}.$$

However, this formulation poses the problem that the state variable $u_h \in V_h$ is not contained in the same Banach space V for all h. In other words, the space for the state variable changes as the parameter h changes. We therefore make the modification of replacing the first equation with

$$A(r_n, g_n) + \partial_g A(r_n, g_n; v_n) = -\frac{1}{2}\varphi_n + \mathcal{D}'\varphi_n + \mathrm{i}k\Big(\lambda \mathcal{S}\varphi_n - \mathrm{Div}(\mu \nabla_\tau \mathcal{S}\varphi_n)\Big) - g_z(\cdot, u_{n-1}; \mathcal{S}\varphi_n) - f$$

and initially calculate an approximation of the state before solving the second equation. Another possibility to circumvent the problem with the different spaces for u_h is to consider the variable-transformed state variable $\widetilde{u}_h = u_h \circ \varphi$, where φ is defined as in (3.1). Note that in order to simultaneously solve the linearized integral equation and the linearized operator equation, we cannot use the updated solution u_n to calculate the domain derivative u_n', but must instead utilize the approximation u_{n-1} determined in the previous iteration.

Since the forward problem is only solved approximately, the idea of an inexact Newton method may come to mind. Motivated by the inexact Newton methods in [DES82] for well-posed problems, Hanke suggested the regularized Levenberg-Marquardt scheme for solving nonlinear inverse problems in [Han97]. The idea was then generalized by Rieder ([Rie99]) and further developed in [LR10]. The idea of the inexact Newton method consists of finding a family of regularized approximations $\{h_n^{(l)}\}$ before updating the boundary curve. More precisely, we can perform l inner iterations such that

$$\|u_\infty^\delta - F(r_n) - F'[r_n]h_n^{(l)}\|_2 \le \eta \|u_\infty^\delta - F(r_n)\|_2\,,$$

for a specified value $\eta \in (0, 1)$. The next iteration is then updated by $r_{n+1} := r_n + h_n^{(l)}$. Again, we must take into account that the state variable $u_h \in V_h$ is not contained in the same Banach space V for all h. We can, however, apply this method to calculate a solution to the forward problem. This means that instead of proceeding directly to the inverse problem after one iteration step in the forward problem, we can first improve the update u_n in several steps and then use this hopefully more accurate approximation to calculate a solution of the inverse problem, see Algorithm 2. We would like to note here that for the numerical examples considered in Chapter 5,

Algorithm 2 Regularized Newton method with l inner iterations

Input: initial guesses u_0^0 and r_0, wave number k, noise level δ.

Output: Approximation of forward problem and far field pattern, update boundary curve.

Set $u_0^0 = u^i$, $r_0 =$ radius circle, $n = 0$.
for $j = 1, 2, \dots, l$ **do**
  Update $\varphi_n^j = \left(-\frac{1}{2}I + \mathcal{D}' + \mathrm{i}k\mathcal{S} - \mathrm{i}k\frac{\mathrm{d}}{\mathrm{d}s}\left(\mu\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{S}\cdot\right) - g_z(\cdot, u_n^{j-1}; \mathcal{S}\cdot)\right)^{-1} f$,
  $u_n^j = \mathcal{S}\varphi_n^j + u^i$.
end for
Set $\varphi_n = \varphi_n^l$, $u_{n+1} = u_n^l$,
Update $\widetilde{\varphi}_n = \left(-\frac{1}{2}I + \mathcal{D}' + \mathrm{i}k\mathcal{S} - \mathrm{i}k\frac{\mathrm{d}}{\mathrm{d}s}\left(\mu\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{S}\cdot\right) - g_z(\cdot, u_{n+1}; \mathcal{S}\cdot)\right)^{-1} \widehat{f}(u_{n+1})$,
  $u'_{n+1,\infty} = \mathrm{e}^{\mathrm{i}\pi/4}/\sqrt{8\pi k}\int_{\partial D_n} \mathrm{e}^{-\mathrm{i}ky\cdot}\widetilde{\varphi}_n(y)\,\mathrm{d}s_y = F'_n[r_n]h_n$,
  $h_n = (F'_n[r_n]^* F'_n[r_n] + \alpha R)^{-1}\left[F'_n[r_n]^*\left(F_n(r_n) - u_\infty^\delta\right)\right]$,
  $r_{n+1} = r_n + \mathrm{Re}\,(h_n)$,
  $n = n + 1$.
if $\|F_n(r_n) - u_\infty^\delta\|_2 \le \tau\delta$ **then**
  Break.
end if

no significant improvement of the results can be observed compared to Algorithm 1.

Further modifications can be made when choosing the regularization method. In this thesis, we employ a Levenberg-Marquardt method, which results from applying Tikhonov regularization to the linearized problem. With a suitable choice for the regularization parameter, this method leads to very accurate reconstructions of the unknown scatterer from the far-field patterns, as we will see in Chapter 5. In our examples, we select the regularization parameter a posteriori. For this purpose, we can either obtain a suitable parameter α by trial and error or, as suggested in [Han97], by using Morozov's discrepancy principle. Since each Newton step involves solving the forward problem for evaluating $F(r)$ and $F'[r]$, an efficient forward solver is required. Additionally, good a priori information must be available in order to select an initial guess that ensures convergence to a global minimum.

Adding a penalty term results in the iteratively regularized Gauss-Newton method introduced by Bakushinskii, see [Bak92]. Here, the approximate solution r_{n+1} minimizes the functional

$$\Phi(r) := \|u_\infty^\delta - F(r_n) - F'[r_n](r - r_n)\|_2 + \alpha_k\|r - r_0\|_2\,,$$

where r_0 is an initial guess for the radial function of the boundary curve. In other words, r_{n+1} minimizes the Tikhonov functional, whereby the nonlinear operator F is linearized around r_n, see [EHN96, Chap. 10]. Beyond this, generalizations of the iteratively regularized Gauss-Newton method may also be considered, see [KNS08, Sec. 4.3].

Another regularization method emerges from considering the fixed point equation

$$r = \Phi(r) := r + F'[r]^*(u_\infty - F(r))$$

for nonlinear problems. By computing successive approximations of this equation, we obtain the nonlinear Landweber iteration, given by

$$r_{n+1} = r_n + F'[r_n]^*(u_\infty^\delta - F(r_n))\,,$$

see [KNS08, Chap. 2]. Motivated by the iteratively regularized Gauss-Newton method, a penalty term can also be added in the case of the Landweber iteration, which leads to the iteratively regularized Landweber iteration. For more details, see [KNS08, Sec. 3.2].

For a comprehensive discussion of various iterative regularization methods and possible convergence results, we refer to the work [KNS08] by Kaltenbacher, Neubauer, and Scherzer and the references therein.

CHAPTER 5

Numerical Examples

The performance of the shape reconstruction algorithm (Alg. 1) presented in Chapter 4 will now be tested on three specific examples in two dimensions. In Section 5.1.1, we first consider noise-free synthetic data before we add 5% equally distributed random noise to the data in Section 5.1.2.

5.1. All-at-once Regularized Newton Method

5.1.1. Noise-free Data

First we consider the reconstruction from synthetic data without noise using the regularized Newton scheme. For the computation of the synthetic data we evaluate 64 discretization points on the boundary curve, while for the inverse scheme, we use 32 discretization points on the boundary with equidistant angles.

Example 5.1. We reconstruct an apple-shaped and a peanut-shaped scattering object with the parameterizations

$$\gamma_{\mathrm{a}}(t) = \frac{0.5 + 0.4\cos(t) + 0.1\sin(2t)}{1 + 0.7\cos(t)}\,(\cos(t), \sin(t))^\top, \quad 0 \le t \le 2\pi,$$

$$\gamma_{\mathrm{p}}(t) = \sqrt{\cos^2(t) + 0.25\sin^2(t)}\,(\cos(t), \sin(t))^\top, \qquad 0 \le t \le 2\pi,$$

and utilize the impedance functions

$$\lambda(\gamma(t)) = \frac{1}{1 - 0.2\sin(2t)} \quad \text{for} \quad 0 \le t \le 2\pi,$$
$$\mu(\gamma(t)) = \frac{1}{1 + 0.3\cos(t)} \quad \text{for} \quad 0 \le t \le 2\pi,$$

where $\gamma \in \{\gamma_{\mathrm{a}}, \gamma_{\mathrm{p}}\}$, as suggested in [Kre18]. We can interpret the impedance functions as given in a neighborhood of ∂D depending only on the polar angle. To approximate the boundary curve, we choose trigonometric polynomials of degree $m = 4$ and consider the wave number $k = 2$.

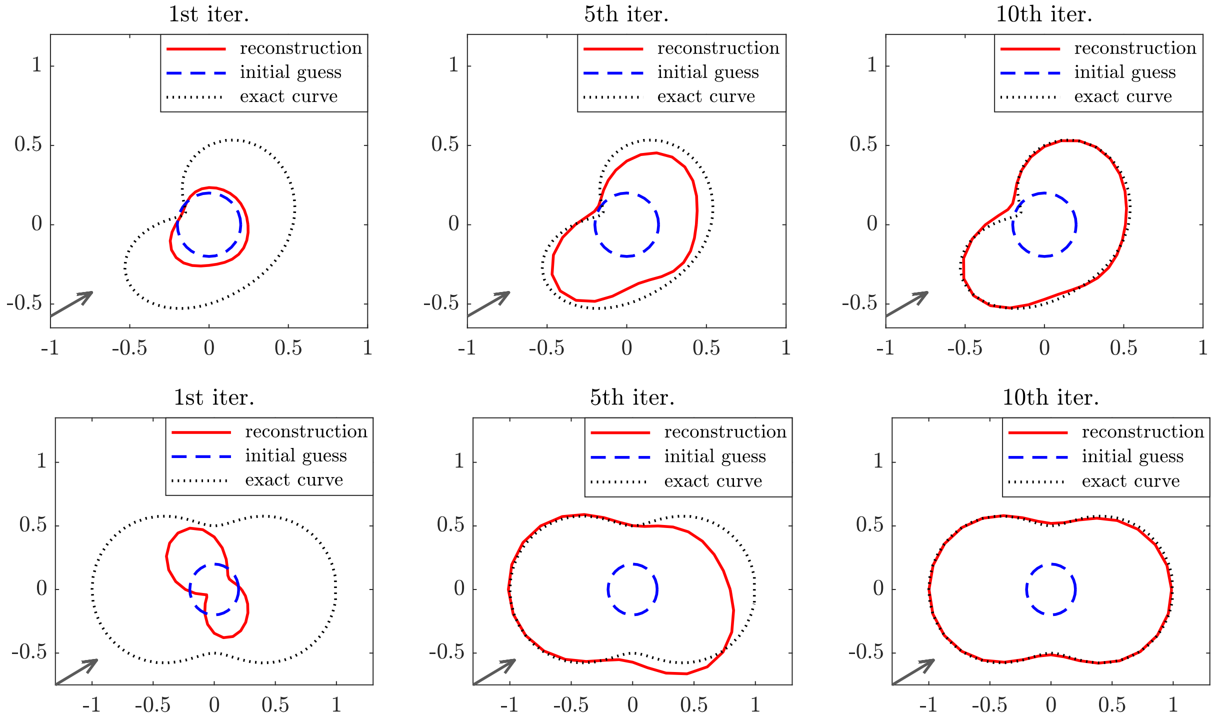

FIGURE 5.1. 1st, 5th and 10th iteration in the case of noise-free data.

In addition, we set the incident field to be a plane wave $u^i(x) = \mathrm{e}^{\mathrm{i}kx\cdot\theta}$, $x \in \mathbb{R}^2$, with incident direction $\theta = \left(\cos(\frac{\pi}{6}), \sin(\frac{\pi}{6})\right)^\top$. As a nonlinear function at the boundary, we specify

$$g(\cdot, u) = u + \sin(u) \quad \text{with} \quad g_z(\cdot, u; z) = (1 + \cos(u))z\,,$$

as in [WR88]. This nonlinearity has the advantage that its linearization g_z is $\mathbb{C}$-linear with respect to z, which means that we do not need a real matrix representation of the boundary integral operator, as presented in Section 2.4.2. Furthermore, we see that the function g_z is uniformly bounded in $u \in \mathbb{C}$, which implies that the corresponding Nemytskii operator is Lipschitz-continuous and strongly monotone, see [WR88] and the references therein.

The angle of the incident plane wave is indicated by an arrow in the lower left corner, the original boundary curve by a dotted line, and the initial guess, a circle with radius $r = 0.2$, by a dashed line. It can be observed that choosing the radius of the circle between $r = 0.08$ and $r = 0.89$ for the apple-shaped object and between $r = 0.2$ and $r = 1.36$ for the peanut-shaped object leads to similar results, possibly with a few more iteration steps.

We have set the regularization parameter here to $\alpha = 9 \cdot 10^{-2}$. Numerical tests show that a wide range of regularization parameters leads to comparable results. However, for the peanut-shaped obstacle, the radius of the initial guess has to be increased in order to choose a smaller regularization parameter. In the case of the apple-shaped object, we find by trial and error that $\alpha = 5 \cdot 10^{-3}$ still provides a meaningful result. If we reduce the wave number to $k = 1$, then $\alpha = 4 \cdot 10^{-7}$ is sufficient. For very large regularization parameters, the reconstruction of the kink deteriorates.

Figure 5.2 shows the relative discrete L^2 errors for both shapes. On the one hand, the

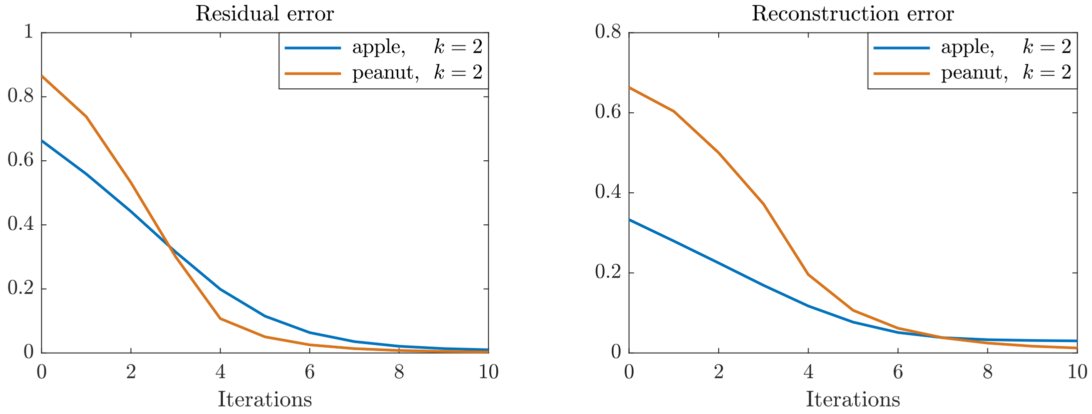

FIGURE 5.2. Relative discrete L^2 errors.

residual error $\|F_n(r_n) - u_\infty^\delta\|_{L^2}/\|u_\infty^\delta\|_{L^2}$ and, on the other hand, the reconstruction error $\|r_n - r_{\text{exact}}\|_{L^2}/\|r_{\text{exact}}\|_{L^2}$. After only 10 iterations, the relative residual error for the apple shape reaches $\text{err}_{\text{res, a}} = 0.0099$ and for the peanut shape we get $\text{err}_{\text{res, p}} = 0.003$, while the reconstruction error for the apple shape is $\text{err}_{\text{rec, a}} = 0.0301$ and for the peanut shape it is $\text{err}_{\text{rec, p}} = 0.0123$.

In Lemma 2.17 and Lemma 2.18, we assumed $|\mu| > 0$ to show the well-posedness of the $\mathbb{R}$-linear scattering problem. If we set $\mu \equiv 0$, the reconstruction is still good, but a deterioration is noticeable. In the case of the apple-shaped object, the kink is reconstructed worse, and in the case of the peanut-shaped object, the radius of the initial guess has to be increased in order to obtain a meaningful reconstruction. This observation is consistent with those in the work [YZZ14] by Yang et al. concerning linear generalized impedance boundary conditions.

Overall, we observe a stable performance for the apple-shaped and peanut-shaped objects in the case of noise-free synthetic data. $\triangle$

Example 5.2. We next consider a garlic-shaped and a kite-shaped object with the parameterizations

$$\gamma_{\text{g}}(t) = \big(1 - \sin(t)\cos^2(t)\big)\big(\cos(t), \sin(t)\big)^\top, \qquad 0 \le t \le 2\pi,$$
$$\gamma_{\text{k}}(t) = \big(\cos(t) + 0.65\cos(2t) - 0.65,\ 1.5\sin(t)\big)^\top, \quad 0 \le t \le 2\pi.$$

Here, the parameterization γ_{g} originates from [YW08] whereas the parameterization γ_{k} was adopted from [Het98b]. The choice of impedance functions in this example is given as follows:

$$\lambda(\gamma_{\text{g}}(t)) = \frac{1-\mathrm{i}}{1 - 0.1\sin(2t)}, \quad \lambda(\gamma_{\text{k}}(t)) = 1.8 + \cos^3(t) + \sin^3(t) \quad \text{for } \ 0 \le t \le 2\pi,$$
$$\mu(\gamma_{\text{g}}(t)) = \sqrt{1 + 0.5\sin(t)}, \quad \mu(\gamma_{\text{k}}(t)) = 1 + \mathrm{i} \qquad \text{for } \ 0 \le t \le 2\pi,$$

where the subscript g refers to the garlic shape and the subscript k to the kite shape. Except for minor changes, the impedance functions are taken from [YZZ14]. To approximate the boundary curve of the garlic shape, we choose trigonometric polynomials of degree $m = 4$ and consider the wave number $k = 2$. For the kite shape, the wave number $k = 1$ and trigonometric polynomials

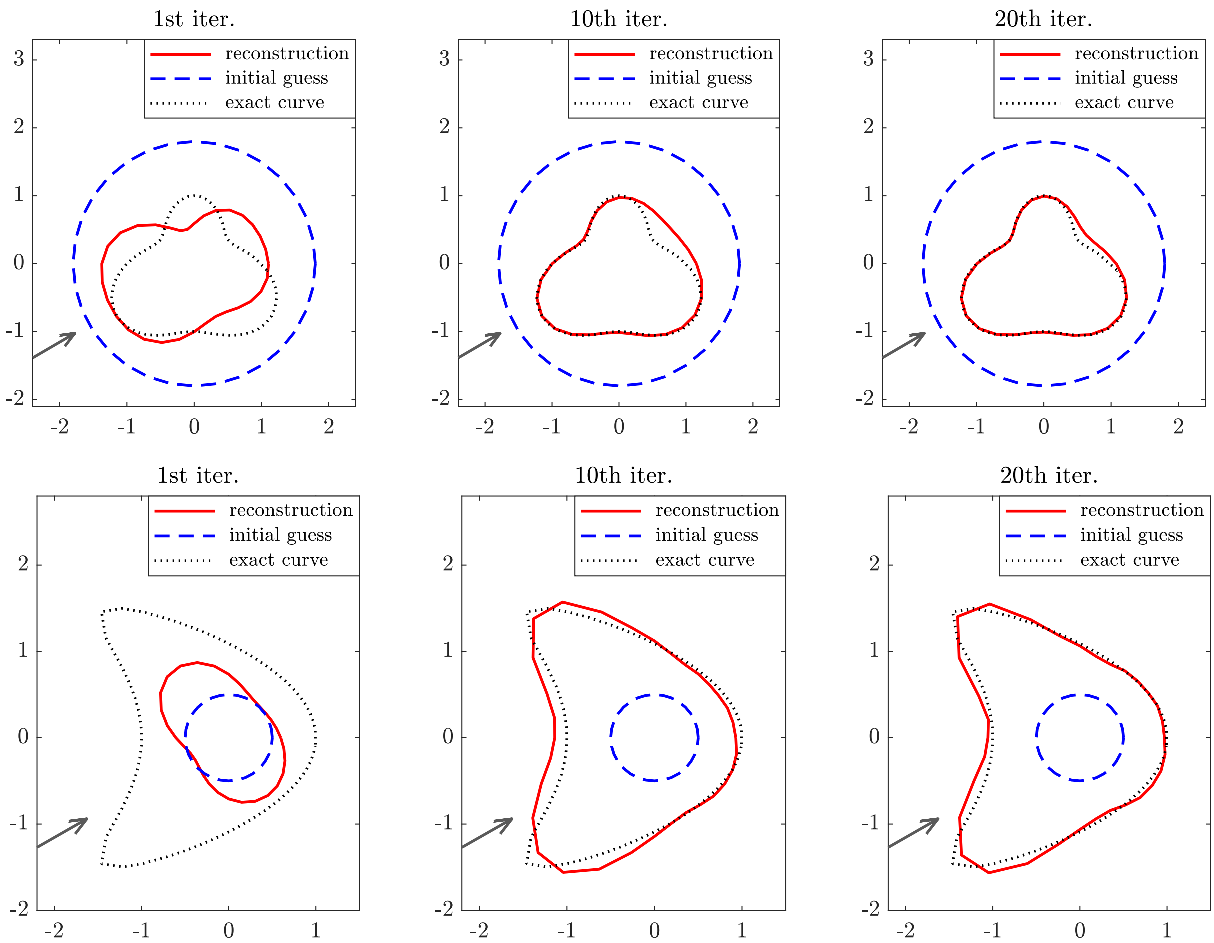

FIGURE 5.3. 1st, 10th and 20th iteration in the case of noise-free data.

of degree $m = 10$ are a more suitable choice. As a nonlinear function at the boundary, we specify

$$g(\cdot, u) = \frac{u}{1 + |u|^2} \quad \text{with} \quad g_z(\cdot, u; z) = \frac{(1 + |u|^2)z - 2\mathrm{Re}(\overline{u}z)u}{(1 + |u|^2)^2},$$

in accordance to Remark 2.8 (i). This nonlinearity is sublinear in u at infinity and fulfills the assumptions of Corollary 2.6. This means that the well-posedness of the direct problem is ensured for this choice of the nonlinearity. However, the linearization g_z is only $\mathbb{R}$-linear, see Example 2.10 (ii). We therefore use the decomposition into real and imaginary parts as given in Example 4.2 (ii).

As initial guesses, we choose a circle with radius $r = 1.8$ for the garlic shape and $r = 0.5$ for the kite shape. Yet for both shapes, a wide range of radii in the initial guess yields a meaningful reconstruction. We set the regularization parameter to $\alpha = 0.4$ here, which may seem high at first sight. However, we can reduce it considerably by decreasing the radius of the initial guess in the case of the garlic shape and increasing it in the case of the kite shape.

If we consider the classical Leontovich boundary conditions, i.e., $\mu \equiv 0$, we observe in this example only a deterioration of the reconstruction for the kite shape, but not for the garlic shape.

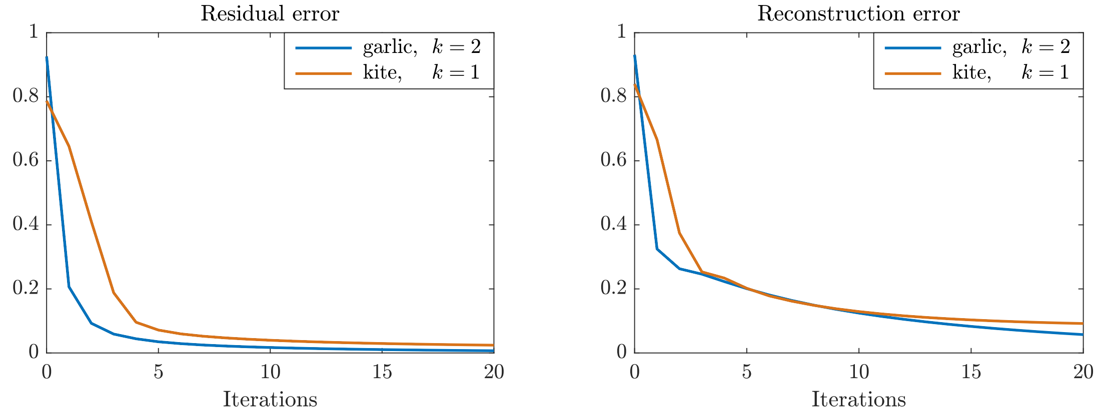

FIGURE 5.4. Relative discrete L^2 errors.

It can be noted that the kite shape is very sensitive to the choice of impedance functions, which is why we have chosen μ to be constant here. However, we are unaware of the reason for this observation.

Figure 5.4 shows for both shapes the relative residual error $\|F_n(r_n) - u_\infty^\delta\|_{L^2}/\|u_\infty^\delta\|_{L^2}$ and the relative reconstruction error $\|r_n - r_{\text{exact}}\|_{L^2}/\|r_{\text{exact}}\|_{L^2}$. After 20 iterations, the relative residual error for the garlic shape reaches $\text{err}_{\text{res, g}} = 0.0069$ and for the kite shape we obtain $\text{err}_{\text{res, k}} = 0.0243$, while the reconstruction error for the garlic shape is $\text{err}_{\text{rec, g}} = 0.0573$ and for the kite shape it is $\text{err}_{\text{rec, k}} = 0.0919$. This example also shows that the reconstruction of the shape using the all-at-once Newton-type method is very accurate when the data is noise-free. △

Example 5.3. We now reconstruct a four-leaf object and a bow tie-shaped object, which are given by the parameterizations

$$\gamma_{\text{l}}(t) = (1 + 0.4\sin(4t))\,(\cos(t), \sin(t))^\top, \qquad 0 \le t \le 2\pi,$$
$$\gamma_{\text{r}}(t) = \sqrt{(0.64\cos(t))^2 + (0.58 \cdot 1.4\sin(t) + 0.58\sin(t)\cos(2t))^2}(\cos(t), \sin(t))^\top, \quad 0 \le t \le 2\pi,$$

where the subscript l refers to the leaf shape and the subscript r to the bow tie shape. The first parameterization is similar to the one used in [HKS09], where we only consider a four-leaf object, since the five-leaf object requires more incident directions for a reasonable reconstruction, see Section 5.1.3. The second parameterization is similar to the one in [AR24], except that we have deepened the notch a little. In this example, the impedance functions are given by

$$\lambda(\gamma_{\text{l}}(t)) = \frac{1-\mathrm{i}}{1 - 0.1\sin(2t)}, \quad \lambda(\gamma_{\text{r}}(t)) = 1 + 0.5\mathrm{i} \qquad \text{for } \; 0 \le t \le 2\pi,$$
$$\mu(\gamma_{\text{l}}(t)) = 0.5(1 + \cos^2(t)), \quad \mu(\gamma_{\text{r}}(t)) = \frac{1}{1 + 0.3\cos(t)} \qquad \text{for } \; 0 \le t \le 2\pi,$$

and as a nonlinear function, we choose the cubic Kerr nonlinearity

$$g(\cdot, u) = |u|^2 u \quad \text{with} \quad g_z(\cdot, u; z) = |u|^2 z + 2\mathrm{Re}(\overline{u}z)u$$

from the illustrative Example 2.2.

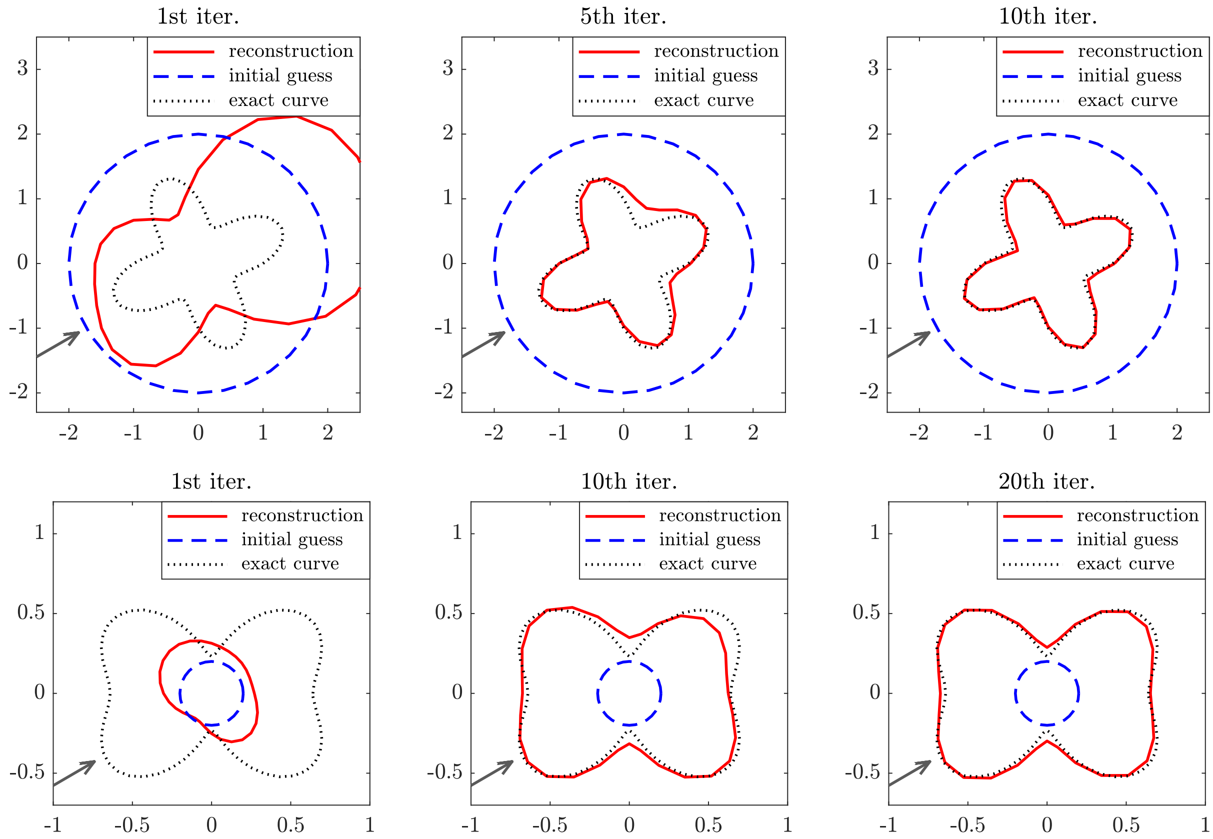

FIGURE 5.5. 1st, 5th/10th and 10th/20th iteration in the case of noise-free data.

Figure 5.5 shows the reconstruction after the 5th and 10th iterations for the leaf-shaped object and after the 10th and 20th iterations for the bow tie-shaped one.

As initial guesses, we choose a circle with radius $r = 2$ for the leaf shape and $r = 0.2$ for the bow tie shape. Alternatively, for a sufficiently good reconstruction, the radii can also be chosen in the range $r_{\text{leaf}} \in [0.3, 2.1]$ for the first and $r_{\text{rib}} \in [0.2, 0.9]$ for the second parameterization.

As in the first example, we use trigonometric polynomials of degree $m = 4$ and consider the wave number $k = 2$. Further, we set the regularization parameter to $\alpha = 0.05$ for the leaf shape and to $\alpha = 0.09$ for the bow tie shape. The regularization parameter can be chosen smaller, where a significantly larger range leads to similar results for the bow tie shape, starting at $\alpha = 4 \cdot 10^{-4}$, in comparison to the leaf shape, where we should use at least $\alpha = 0.03$.

It can be observed that the choice of the impedance function μ is crucial for the leaf shape. While for $\mu \equiv 0$ a reconstruction of the shape with the selected parameters is not possible, the functions $\mu(t) = 1/(1 + 0.3\cos(t))$, $t \in [0, 2\pi]$, from Example 5.1 and $\mu(t) = \sqrt{1 + 0.5\sin(t)}$, $t \in [0, 2\pi]$, from Example 5.2 lead to worse results. Conversely, the bow tie shape is much more robust with respect to the choice of μ. However, a deterioration can also be observed here in the case of $\mu \equiv 0$.

Figure 5.6 shows the relative residual error as well as the relative reconstruction error for both shapes. For the leaf shape, after 10 iterations, the relative residual error is $\text{err}_{\text{res},1} = 0.0273$ and

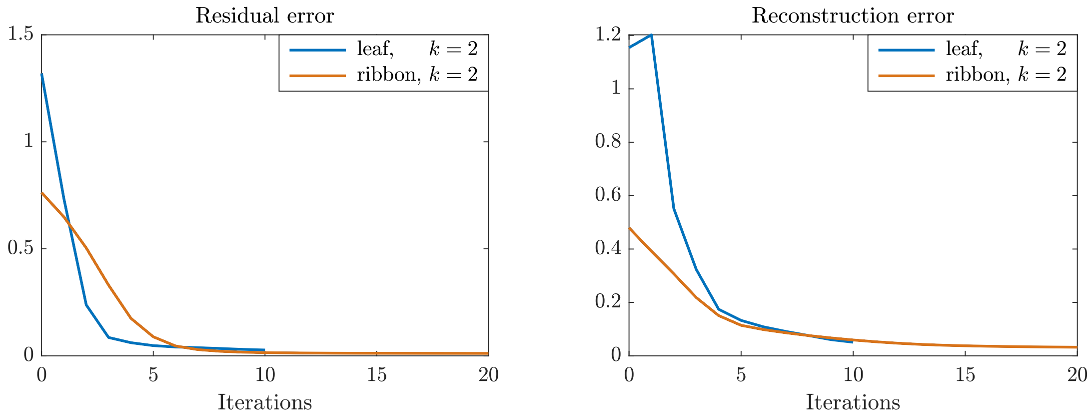

Figure 5.6. Relative discrete L^2 errors.

the relative reconstruction error is $\mathrm{err}_{\mathrm{rec,\,l}} = 0.0509$. After 20 iterations, the relative residual error for the bow tie shape reaches the value $\mathrm{err}_{\mathrm{res,\,r}} = 0.0114$ and the relative reconstruction error is $\mathrm{err}_{\mathrm{rec,\,r}} = 0.0322$. △

In summary, we can say that in all three examples, we achieve a promising reconstruction after only a few iterations, provided that no noise is added to the data. Here, both the regularization parameters and the radii of the initial guesses can be chosen from a wide range. A suitable choice for the impedance functions λ and μ, which can have a major influence on the reconstruction, is somewhat more challenging for some scattered objects, such as the kite shape or the bow tie shape.

5.1.2. Noisy Data

Now we add equally distributed random noise to the data at the grid points. The performance of the regularized all-at-once Newton method is illustrated by displaying the best, the mean, and the worst results in terms of the error in the approximated boundary curve from 100 experiments. For the computation of the synthetic data, we evaluate 64 discretization points on the boundary curve, whereas for the inverse scheme, we use 32 discretization points on the boundary with equidistant angles. In all examples presented, we use one plane wave $u^i(x) = \mathrm{e}^{\mathrm{i}kx\cdot\theta}$, $x \in \mathbb{R}^2$, as incident field with incident direction $\theta = \big(\cos(\frac{\pi}{6}), \sin(\frac{\pi}{6})\big)^\top$. For the sake of comparability of the results, we consider the same scattering obstacles as in the noise-free case. The degrees of the trigonometric polynomials are kept the same, whereas the regularization parameters must be increased in order to obtain meaningful reconstructions.

Example 5.4. We add 5% equally distributed random noise to the data and consider reconstructions of the apple- and peanut-shaped obstacles with parameterizations, impedance functions, and nonlinearity as in Example 5.1. Note that we have set the radius of the initial guess for the peanut shape to $r = 0.3$, instead of $r = 0.2$ as in Example 5.1, so that the iteration does not terminate too early. In the case of noisy data, the regularization parameter has to be increased. Here, we set the regularization parameter to $\alpha = 2$, which turned out to be sufficient in all tests performed. Note that overestimating the required regularization of the linearized equation generally comes at the cost of slowing down the procedure, while underestimating it leads to

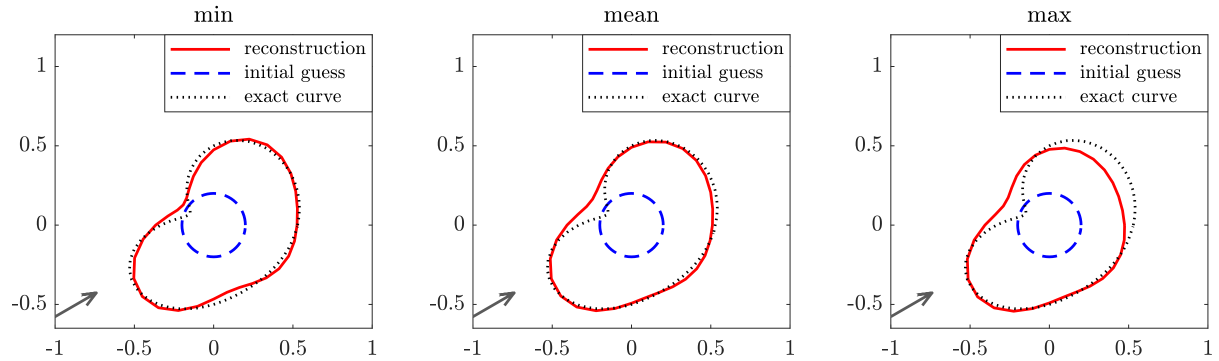

FIGURE 5.7. Reconstruction with 5% noise after 10 iterations.

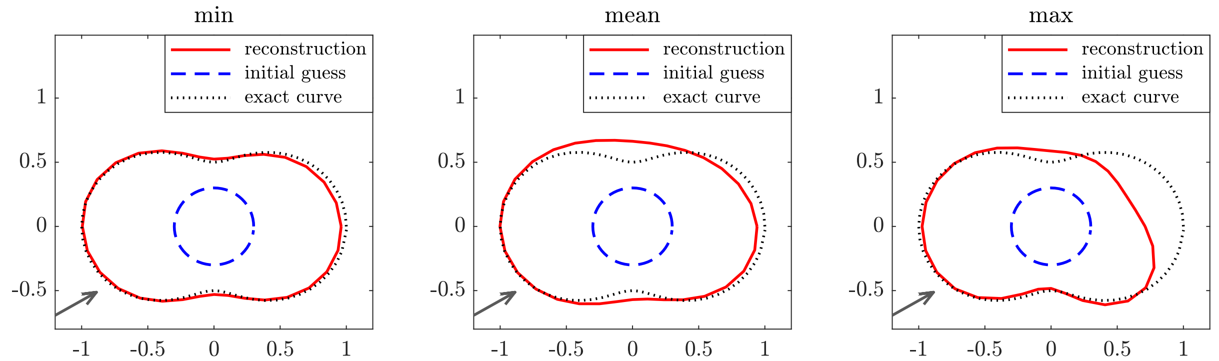

FIGURE 5.8. Reconstructions with 5% noise after 15 iterations.

divergent behavior, see [Het99]. The discrepancy principle (4.10) with $\tau = 1.3$ was used as a stopping criterion, i.e.,

$$\|F_n(r_n) - u_\infty^\delta\| \leq \tau\delta = 1.3 \cdot 0.05 = 0.065\,.$$

Choosing the optimal value for τ is challenging. If τ is smaller than the optimum, the iteration may not be finished before the approximations begin to diverge. However, if the value for τ is chosen larger than the optimum, the iteration may be stopped before the best possible reconstruction is achieved. With $\tau = 1.3$, we are in the second scenario, meaning that 10 iterations are computed for the apple-shaped object and 15 iterations for the peanut-shaped object without the stopping criterion being reached. However, we have only specified a small number of iteration steps here. If we increase the number of steps, the first case occurs, i.e., the iteration terminates prematurely.

The best (min), mean, and worst (max) results from running 100 experiments are shown in Figure 5.7 and Figure 5.8. It can be observed that the reconstructions in the shadow region, which is not illuminated by the incident wave, deteriorate. An improvement of the results might be achieved by adding one or two incident waves. △

Example 5.5. Next, we revisit Example 5.2 in the case of noisy data. We increase the regularization parameter here to $\alpha = 1.8$, which is sufficient for both the garlic shape and the kite shape. As a stopping criterion, we used the discrepancy principle (4.10) with $\tau = 1.3$.

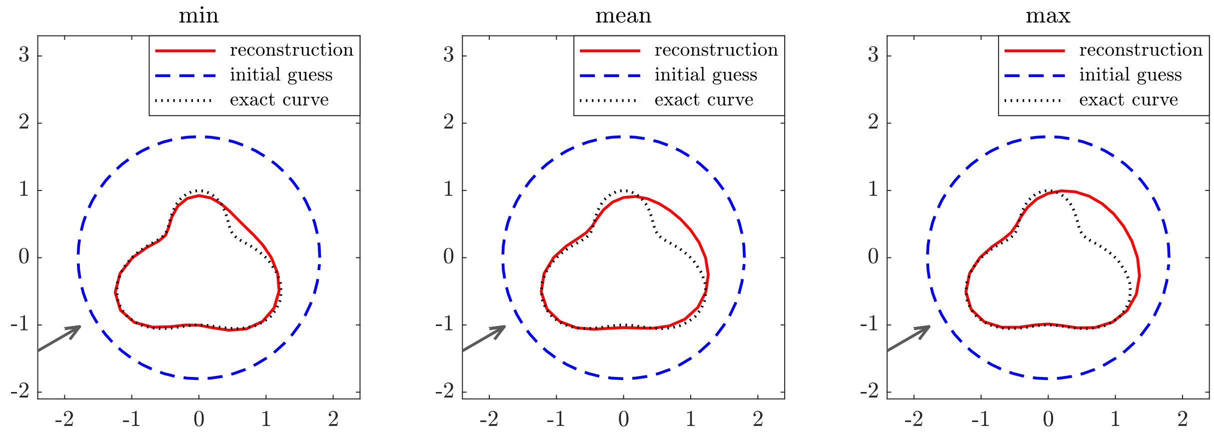

FIGURE 5.9. Reconstructions with 5% noise after 15 iterations.

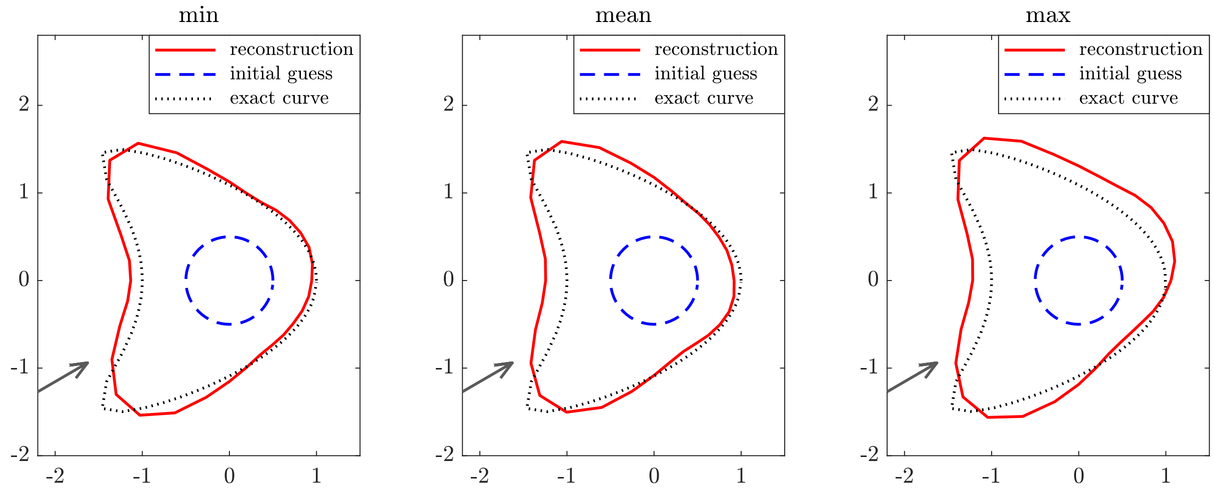

FIGURE 5.10. Reconstructions with 5% noise after 20 iterations.

The best (min), mean, and worst (max) results from 100 experiments are shown in Figure 5.9 and Figure 5.10. Particularly in the case of the garlic shape, it can be observed that the reconstructions become less accurate in the area that is not illuminated by the incident wave.

In this example, the residual error does not fall below the noise level $\delta = 0.05$ in the tests performed. This means that even better results can be achieved with a suitable choice of parameters. However, for the garlic shape, the residual error reaches a value of approximately $\mathrm{err}_{\mathrm{res,\,g}} \approx 0.065$, which is already very close to the 5% threshold. For the kite shape, the residual error is approximately $\mathrm{err}_{\mathrm{res,\,k}} \approx 0.075$. As shown in Figure 5.9 and Figure 5.10, the reconstructions are still very acceptable when 5% noise is added. Due to the difficulty of selecting the appropriate impedance functions in the case of the kite shape, the reconstruction is also somewhat less accurate than for the garlic shape. Note that with 10% noise, no meaningful reconstruction can be achieved with the parameters used here. $\triangle$

Example 5.6. Now, let us revisit Example 5.3 in the case of noisy data. Here, we increase the regularization parameter to $\alpha = 1.8$ for the leaf shape and to $\alpha = 2$ for the bow tie shape. As a stopping criterion, we again use the discrepancy principle (4.10) with $\tau = 1.3$.

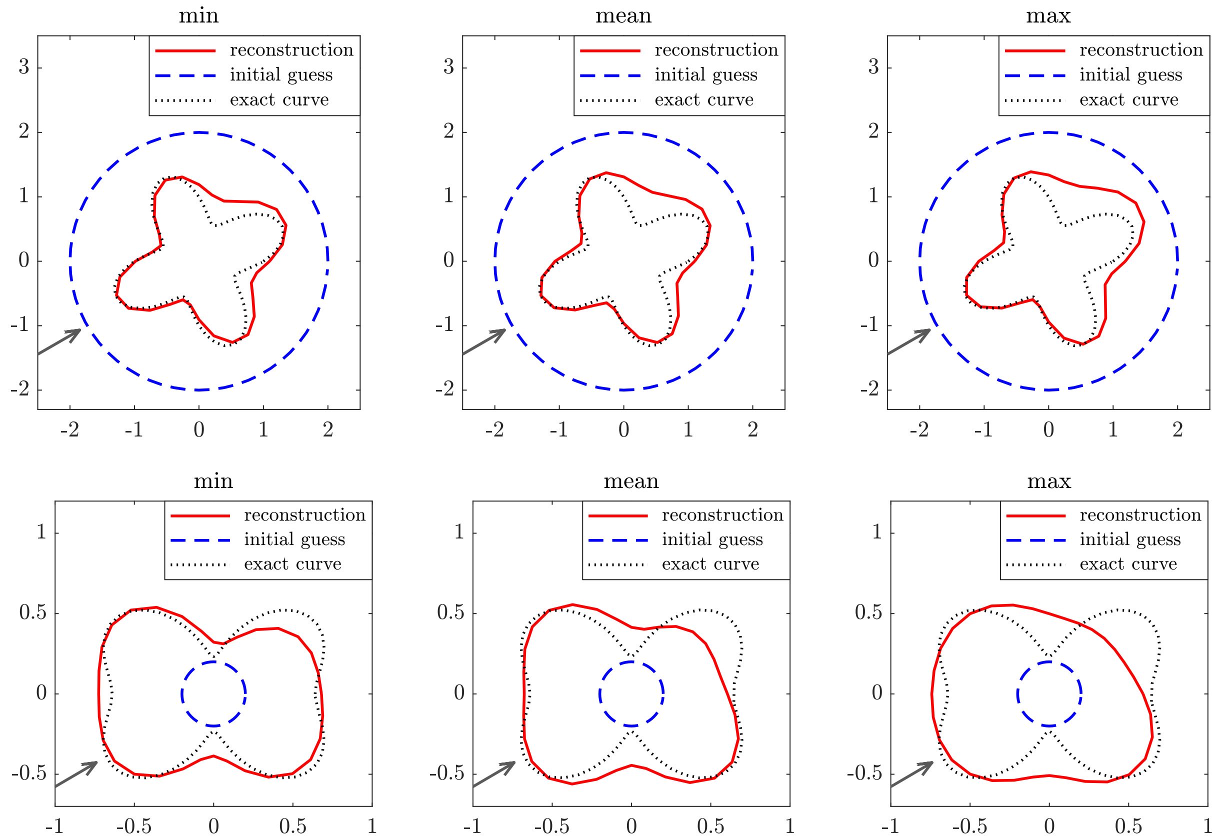

FIGURE 5.11. Reconstructions with 5% noise after 20 iterations.

The best (min), mean, and worst (max) results from 100 experiments are shown in Figure 5.11. While the three reconstruction results for the leaf shape look very similar, a clear deterioration from the best to the worst result can be seen in the case of the bow tie shape.

For the leaf shape, the relative residual error reaches a value of approximately $\mathrm{err}_{\mathrm{res,\,l}} \approx 0.082$, which may be due to the deep indentations. For the bow tie shape, the relative residual error is approximately $\mathrm{err}_{\mathrm{res,\,r}} \approx 0.075$. As shown in Figure 5.11, the reconstructions for the leaf shape are quite good, while the bow tie shape has not been reconstructed particularly well. △

5.1.3. DISTINCT INCIDENT FIELDS

A common way to improve reconstructions from noisy data is to use more than one incident direction for the plane wave u^i or to increase the number of nodal points for the inverse scheme. For example, if we want to reconstruct a leaf shape as in Example 5.6, which has more than four leaves, one incident wave is not sufficient to obtain a meaningful reconstruction.

Example 5.7. In order to obtain the parameterization of a five-leaf shape, we simply need to replace the term $\sin(4\cdot)$ by $\sin(5\cdot)$ in the parameterization of the four-leaf shape, i.e.,

$$\gamma_{l5}(t) = (1 + 0.4\sin(5t))\,(\cos(t), \sin(t))^\top, \quad 0 \le t \le 2\pi.$$

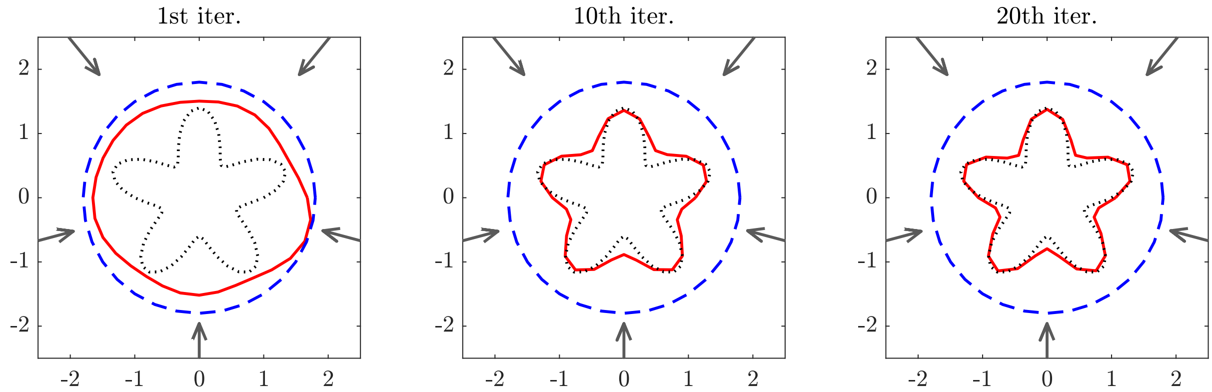

Figure 5.12. 1st, 10th and 20th iteration in the case of noise-free data and $n = 32$ nodal points.

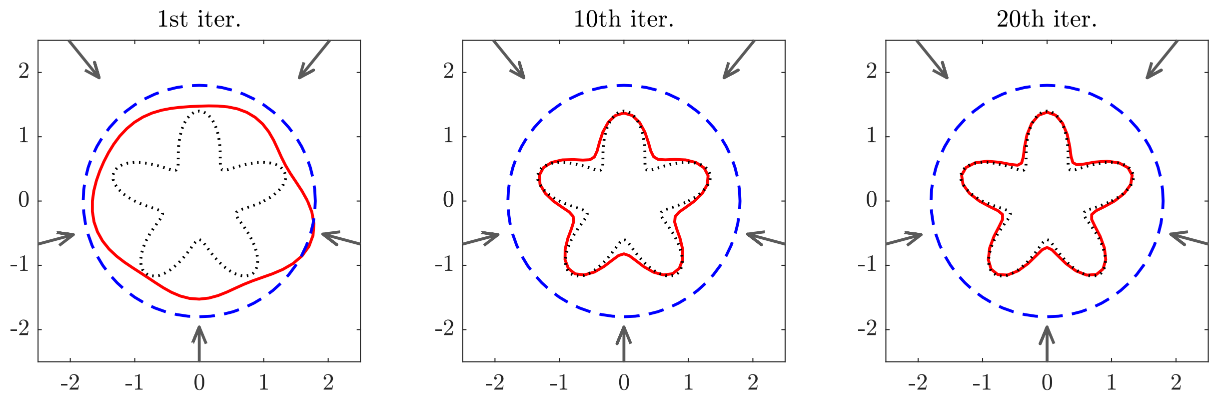

Figure 5.13. 1st, 10th and 20th iteration in the case of noise-free data and $n = 64$ nodal points.

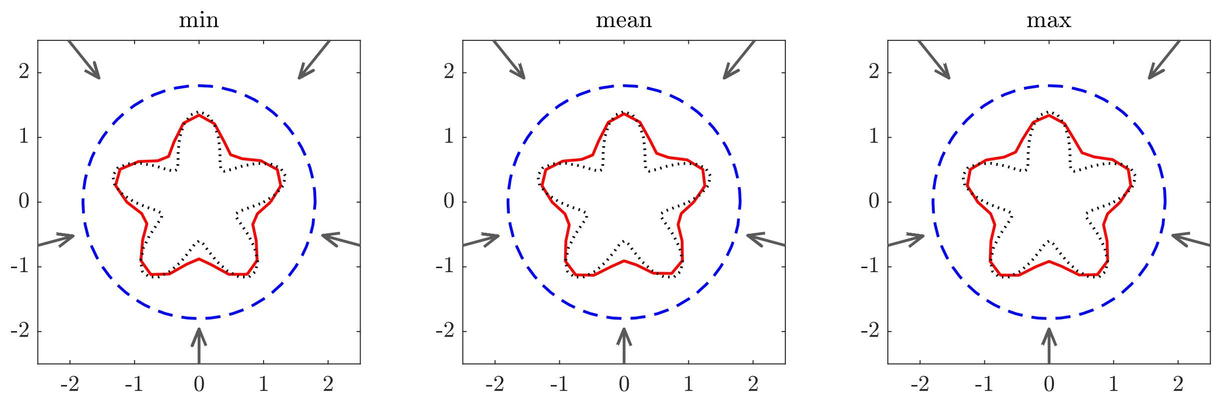

Figure 5.14. Reconstructions with 5% noise after 20 iterations and $n = 32$ nodal points.

We consider the same impedance functions as in Example 5.3, which are given by

$$\lambda(\gamma_{15}(t)) = \frac{1 - \mathrm{i}}{1 - 0.1\sin(2t)} \quad \text{and} \quad \mu(\gamma_{15}(t)) = 0.5(1 + \cos^2(t)) \quad \text{for} \quad 0 \le t \le 2\pi,$$

and as a nonlinear function, we again choose the cubic Kerr nonlinearity

$$g(\cdot, u) = |u|^2 u \quad \text{with} \quad g_z(\cdot, u; z) = |u|^2 z + 2\mathrm{Re}(\overline{u} z) u \, .$$

To approximate the boundary curve of the shape, we choose trigonometric polynomials of degree $m = 6$ and consider the wave number $k = 2$. For noise-free synthetic data, we set the regularization parameter to $\alpha = 0.4$ and increase it to $\alpha = 1.8$ in the case of noisy data.

If we take an incident direction with the appropriate angle for each notch, the reconstructions are more promising for both noise-free data and data with 5% noise added. Figures 5.12 – 5.14 show the reconstruction of a five-leaf shape with five incident directions, indicated by arrows. The first figure displays the reconstructions after 10 and 20 iterations in the case of noise-free synthetic data and $n = 32$ discretization points for the inverse scheme. If we double the number of nodal points, the reconstructions are significantly improved, see Figure 5.13. When 5% noise is added to the data, no discernible difference between the best, mean, and worst results can be observed from running 100 experiments, see Figure 5.14. △

5.2. Conclusion

The examples presented provide a small overview of the performance of the all-at-once regularized Newton-type method introduced in Chapter 4. Modifications to the regularization method were discussed in Section 4.7, but further considerations can also be made in this section. Improvements in the reconstructions may be achieved by selecting more suitable impedance functions or regularization parameters. Beyond that, the choice of initial guess and the number of incident directions also play a decisive role in the effectiveness of the reconstruction algorithm.

In conclusion, we can state that the performance of the presented all-at-once regularized Newton method for acoustic scattering problems with nonlinear generalized impedance boundary conditions is satisfactory in all tested examples and comparable to the well-known linear cases.

APPENDIX A

Derivation of the Boundary Condition

If the field exhibits no variation along the axis of the scattering object, the Laplacian with respect to (s,n) is given by

$$\Delta_{(s,n)} = \partial_n^2 + \kappa(s,n)\partial_n + \left(\frac{1}{1+\kappa(s,0)n}\partial_s\right)^2 , \tag{A.1}$$

see [AH98]. In the thin film, u is a solution to the Helmholtz equation

$$\Delta_{(s,n)}u(s,n) + \omega^2\epsilon_1\left[\mu_1(s,n) + \alpha(s,n)|u(s,n)|^2\right]u(s,n) = 0.$$

Inserting the representation (A.1) of $\Delta_{(s,n)}$ leads to

$$\left(\partial_n^2 + \kappa(s,n)\partial_n + \left(\frac{1}{1+\kappa(s,0)n}\partial_s\right)^2\right)u(s,n) + \omega^2\epsilon_1\left[\mu_1(s,n) + \alpha(s,n)|u(s,n)|^2\right]u(s,n) = 0.$$

Using the extensions (2.7) and (2.8) of $u(s,n;\delta)$ and $\kappa(s,\delta\tau)$ results in

$$\begin{aligned}
&\left(\delta^{-2}\partial_\tau^2 + \delta^{-1}(\kappa(s,0) + \delta\tau\kappa'(s,0) + \ldots)\partial_\tau\right)(u^{(0)}(s,\tau) + \delta u^{(1)}(s,\tau) + \delta^2u^{(2)}(s,\tau) + \ldots)\\
&+ \left(\partial_s^2 - \delta[2\kappa(s,0)\tau\partial_s^2 + \partial_s\kappa(s,0)\tau\partial_s] + \ldots\right)(u^{(0)}(s,\tau) + \delta u^{(1)}(s,\tau) + \delta^2u^{(2)}(s,\tau) + \ldots)\\
&+ \left(\omega^2\epsilon_1\left[\mu_1(s,\tau) + \alpha(s,\tau)|u^{(0)}(s,\tau) + \delta u^{(1)}(s,\tau) + \ldots|^2\right]\right)(u^{(0)}(s,\tau) + \delta u^{(1)}(s,\tau) + \ldots)\\
&= 0.
\end{aligned}$$

Rearranging the coefficients of $\delta^{-2}, \delta^{-1}, \delta^0$ and δ^1 yields

$$\begin{aligned}
&\delta^{-2}\left(\partial_\tau^2u^{(0)}\right) + \delta^{-1}\left(\partial_\tau^2u^{(1)} + \kappa(s,0)\partial_\tau u^{(0)}\right) + \delta^0\Big(\partial_\tau^2u^{(2)} + \kappa(s,0)\partial_\tau u^{(1)} + \tau\kappa'(s,0)\partial_\tau u^{(0)}\\
&+ \partial_s^2u^{(0)} + \omega^2\epsilon_1\left[\mu_1 + \alpha|u^{(0)}|^2\right]u^{(0)}\Big) + \delta\Big(\partial_\tau^2u^{(3)} + \kappa(s,0)\partial_\tau u^{(2)} + \tau\kappa'(s,0)\partial_\tau u^{(1)}\\
&+ \frac{\tau^2}{2}\kappa''(s,0)\partial_\tau u^{(0)} + \partial_s^2u^{(1)} - \left[2\kappa(s,0)\tau\partial_s^2 + \partial_s\kappa(s,0)\tau\partial_s\right]u^{(0)} + \omega^2\epsilon_1\mu_1u^{(1)}\\
&+ \omega^2\epsilon_1\alpha\left[|u^{(0)}|^2u^{(1)} + \left(u^{(0)}\right)^2\overline{u}^{(1)}\right]\Big) + \ldots = 0.
\end{aligned}$$

Comparison of coefficients leads to four differential equations that we can solve by integration. First, we consider the coefficient of δ^{-2} for which

$$\partial_\tau^2 u^{(0)}(s,\tau) = 0$$

holds. Integration provides $\partial_\tau u^{(0)}(s,\tau) = C(s)$ with a constant C depending on s. However, with the boundary condition $\partial_\tau u^{(0)}(s,0) = 0$ we can conclude that $C(s) = 0$ is valid. Therefore,

$$\partial_\tau u^{(0)}(s,\tau) = 0 \quad \text{and} \quad u^{(0)}(s,\tau) = C_0(s)$$

for a constant $C_0(s)$.

We proceed with the coefficient of δ^{-1}, for which we have

$$\partial_\tau^2 u^{(1)}(s,\tau) = -\kappa(s,0)\partial_\tau^2 u^{(0)}(s,\tau) = 0.$$

Again, integrating and exploiting the boundary condition $\partial_\tau u^{(1)}(s,0) = 0$ leads to

$$\partial_\tau u^{(1)}(s,\tau) = 0$$

and thus we get $u^{(1)}(s,\tau) = C_1(s)$ for a constant C_1 depending on s.

For the coefficient of δ^0, we obtain the following identity

$$\begin{aligned}
\partial_\tau^2 u^{(2)}(s,\tau) &= -\kappa(s,0)\partial_\tau u^{(1)} - \tau\kappa'(s,0)\partial_\tau u^{(0)} - \partial_s^2 u^{(0)} - \omega^2\epsilon_1\mu_1 u^{(0)} - \omega^2\epsilon_1\alpha|u^{(0)}|^2 u^{(0)} \\
&= -\partial_s^2 u^{(0)} - \omega^2\epsilon_1\mu_1 u^{(0)} - \omega^2\epsilon_1\alpha|u^{(0)}|^2 u^{(0)}
\end{aligned}$$

and by integrating once we have

$$\partial_\tau u^{(2)}(s,\tau) = -\tau\partial_s^2 u^{(0)} - \omega^2\epsilon_1 u^{(0)}\int_0^\tau \mu_1(s,\tau_1)\,\mathrm{d}\tau_1 - \omega^2\epsilon_1|u^{(0)}|^2u^{(0)}\int_0^\tau \alpha(s,\tau_1)\,\mathrm{d}\tau_1 + C(s).$$

Due to the boundary condition $\partial_\tau u^{(2)}(s,0) = 0$, the constant $C(s)$ vanishes. Integrating a second time results in

$$\begin{aligned}
u^{(2)}(s,\tau) = -\frac{\tau^2}{2}\partial_s^2 u^{(0)} &- \omega^2\epsilon_1 u^{(0)}\int_0^\tau\int_0^{\tau_1}\mu_1(s,\tau_2)\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1 \\
&- \omega^2\epsilon_1|u^{(0)}|^2u^{(0)}\int_0^\tau\int_0^{\tau_1}\alpha(s,\tau_2)\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1 + C_2(s).
\end{aligned}$$

Lastly, we take a look at the coefficient of δ. This is given by

$$\begin{aligned}
\partial_\tau^2 u^{(3)} &= -\kappa(s,0)\partial_\tau u^{(2)} - \tau\kappa'(s,0)\partial_\tau u^{(1)} - \frac{\tau^2}{2}\kappa''(s,0)\partial_\tau u^{(0)} - \partial_s^2 u^{(1)} + 2\kappa(s,0)\tau\partial_s^2 u^{(0)} \\
&\quad + \partial_s\kappa(s,0)\tau\partial_s u^{(0)} - \omega^2\epsilon_1\mu_1 u^{(1)} - \omega^2\epsilon_1\alpha\left[|u^{(0)}|^2u^{(1)} + \left(u^{(0)}\right)^2\overline{u}^{(1)}\right] \\
&= \kappa(s,0)\tau\partial_s^2 u^{(0)} + \kappa(s,0)\omega^2\epsilon_1 u^{(0)}\int_0^\tau \mu_1(s,\tau_1)\,\mathrm{d}\tau_1 + \kappa(s,0)\omega^2\epsilon_1|u^{(0)}|^2u^{(0)}\int_0^\tau \alpha(s,\tau_1)\,\mathrm{d}\tau_1 \\
&\quad - \partial_s^2 u^{(1)} + 2\kappa(s,0)\tau\partial_s^2 u^{(0)} + \partial_s\kappa(s,0)\tau\partial_s u^{(0)} - \omega^2\epsilon_1\mu_1 u^{(1)}
\end{aligned}$$

$$- \omega^2 \epsilon_1 \alpha \left[|u^{(0)}|^2 u^{(1)} + \left(u^{(0)}\right)^2 \overline{u}^{(1)} \right].$$

By integrating, once we obtain

$$\begin{aligned}
\partial_\tau u^{(3)} = \kappa(s,0) \frac{\tau^2}{2} \partial_s^2 u^{(0)} + \kappa(s,0) \omega^2 \epsilon_1 u^{(0)} \int_0^\tau \int_0^{\tau_1} \mu_1(s,\tau_2) \, \mathrm{d}\tau_2 \, \mathrm{d}\tau_1 \\
+ \kappa(s,0) \omega^2 \epsilon_1 |u^{(0)}|^2 u^{(0)} \int_0^\tau \int_0^{\tau_1} \alpha(s,\tau_2) \, \mathrm{d}\tau_2 \, \mathrm{d}\tau_1 - \tau \partial_s^2 u^{(1)} + \kappa(s,0) \tau^2 \partial_s^2 u^{(0)} \\
+ \frac{1}{2} \partial_s \kappa(s,0) \tau^2 \partial_s u^{(0)} - \omega^2 \epsilon_1 u^{(1)} \int_0^\tau \mu_1(s,\tau_1) \, \mathrm{d}\tau_1 \\
- \omega^2 \epsilon_1 \left[|u^{(0)}|^2 u^{(1)} + \left(u^{(0)}\right)^2 \overline{u}^{(1)} \right] \int_0^\tau \alpha(s,\tau_1) \, \mathrm{d}\tau_1 + C(s)
\end{aligned}$$

and again it follows from the boundary condition $\partial_\tau u^{(3)}(s,0) = 0$ that $C(s) = 0$. Integrating a second time leads to

$$\begin{aligned}
u^{(3)}(s,\tau) = \kappa(s,0) \frac{\tau^3}{6} \partial_s^2 u^{(0)} + \kappa(s,0) \omega^2 \epsilon_1 u^{(0)} \int_0^\tau \int_0^{\tau_1} \int_0^{\tau_2} \mu_1(s,\tau_3) \, \mathrm{d}\tau_3 \, \mathrm{d}\tau_2 \, \mathrm{d}\tau_1 \\
+ \kappa(s,0) \omega^2 \epsilon_1 |u^{(0)}|^2 u^{(0)} \int_0^\tau \int_0^{\tau_1} \int_0^{\tau_2} \alpha(s,\tau_3) \, \mathrm{d}\tau_3 \, \mathrm{d}\tau_2 \, \mathrm{d}\tau_1 - \frac{\tau^2}{2} \partial_s u^{(1)} \\
+ \kappa(s,0) \frac{\tau^2}{2} \partial_s^2 u^{(0)} + \frac{1}{6} \partial_s \kappa(s,0) \tau^3 \partial_s u^{(0)} - \omega^2 \epsilon_1 u^{(1)} \int_0^\tau \int_0^{\tau_1} \mu_1(s,\tau_2) \, \mathrm{d}\tau_2 \, \mathrm{d}\tau_1 \\
- \omega^2 \epsilon_1 \left[|u^{(0)}|^2 u^{(1)} + \left(u^{(0)}\right)^2 \overline{u}^{(1)} \right] \int_0^\tau \int_0^{\tau_1} \alpha(s,\tau_2) \, \mathrm{d}\tau_2 \, \mathrm{d}\tau_1 + C_3(s).
\end{aligned}$$

Now we insert the calculated derivatives up to the third order into the asymptotic expansion (2.10) and sort the individual terms in order to obtain

$$\begin{aligned}
&\frac{1}{\delta} \Big(\partial_\tau u^{(0)} + \delta \partial_\tau u^{(1)} + \delta^2 \partial_\tau u^{(2)} + \delta^3 \partial_\tau u^{(3)} \Big) \\
&= \delta \Big[-\tau \partial_s^2 u^{(0)} - \omega^2 \epsilon_1 u^{(0)} \int_0^\tau \mu_1(s,\tau_1) - |u^{(0)}|^2 \alpha(s,\tau_1) \, \mathrm{d}\tau_1 \Big] \\
&\quad + \delta^2 \Big[\kappa(s,0) \frac{\tau^2}{2} \partial_s^2 u^{(0)} + \kappa(s,0) \omega^2 \epsilon_1 u^{(0)} \int_0^\tau \int_0^{\tau_1} \mu_1(s,\tau_2) + |u^{(0)}|^2 \alpha(s,\tau_2) \, \mathrm{d}\tau_2 \, \mathrm{d}\tau_1 \\
&\quad - \tau \partial_s^2 u^{(1)} + \kappa(s,0) \tau^2 \partial_s^2 u^{(0)} + \frac{1}{2} \partial_s \kappa(s,0) \tau^2 \partial_s u^{(0)} - \omega^2 \epsilon_1 u^{(1)} \int_0^\tau \mu_1(s,\tau_1) \, \mathrm{d}\tau_1 \\
&\quad - \omega^2 \epsilon_1 \left[|u^{(0)}|^2 u^{(1)} + (u^{(0)})^2 \overline{u}^{(1)} \right] \int_0^\tau \alpha(s,\tau_1) \, \mathrm{d}\tau_1 \Big] \\
&= -\delta \tau \partial_s^2 \left(u^{(0)} + \delta u^{(1)} \right) - \omega^2 \epsilon_1 \delta \left(u^{(0)} + \delta u^{(1)} \right) \int_0^\tau \mu_1(s,\tau_1) \, \mathrm{d}\tau_1 \\
&\quad - \omega^2 \epsilon_1 \delta \left(|u^{(0)}|^2 u^{(0)} + \delta |u^{(0)}|^2 u^{(1)} + \delta (u^{(0)})^2 \overline{u}^{(1)} \right) \int_0^\tau \alpha(s,\tau_1) \, \mathrm{d}\tau_1 \\
&\quad + \kappa(s,0) \omega^2 \epsilon_0 \delta^2 u^{(0)} \int_0^\tau \int_0^{\tau_1} \mu_1(s,\tau_2) + |u^{(0)}|^2 \alpha(s,\tau_2) \, \mathrm{d}\tau_2 \, \mathrm{d}\tau_1 \\
&\quad + \frac{1}{2} \tau^2 \delta^2 \underbrace{\left(\kappa(s,0) \partial_s^2 u^{(0)} + \partial_s \kappa(s,0) \partial_s u^{(0)} \right)}_{\partial_s \left(\kappa(s,0) \partial_s u^{(0)} \right)} + \kappa(s,0) \tau^2 \delta^2 \partial_s^2 u^{(0)}.
\end{aligned}$$

Evaluating at $\tau = 1$ and using the expansion of u provides

$$\begin{aligned}\partial_n u = &-\omega^2 \epsilon_1 \delta u \int_0^1 \mu_1(s,\tau) + |u|^2 \alpha(s,\tau) \,\mathrm{d}\tau \\ &+ \kappa(s,0)\omega^2 \epsilon_1 \delta^2 u \int_0^1 \int_0^\tau \mu_1(s,\tau_1) + |u|^2 \alpha(s,\tau_1) \,\mathrm{d}\tau_1 \,\mathrm{d}\tau \\ &+ \frac{1}{2}\delta^2 \partial_s \left(\kappa(s,0)\partial_s u\right) - \delta \partial_s^2 u + \delta^2 \kappa(s,0)\partial_s^2 u.\end{aligned}$$

Therefore, an effective boundary condition for the scattering problem of a perfectly conducting obstacle covered by a nonlinear thin layer is given by

$$\begin{aligned}\partial_n u + \omega^2 \epsilon_1 \delta \left[\tilde{\mu_1} - \delta\kappa(s,0)\tilde{\tilde{\mu_1}}\right] u - \partial_s \left(\left[\frac{1}{2}\delta^2 \kappa(s,0) - \delta\right] \partial_s u \right) + \delta^2 \kappa(s,0) \partial_s^2 u \\ = \omega^2 \epsilon_1 \delta \left[\delta \kappa(s,0)\tilde{\tilde{\alpha}} - \tilde{\alpha}\right] |u|^2 u.\end{aligned}$$

APPENDIX B

Matrix Representation - Synthetic Data

For the synthetic data, we consider the boundary integral equation $\mathcal{B}u_n = f$, defined in (4.17). The operator $\mathcal{B}$ in the discrete sense is given by

$$\mathcal{B}\widetilde{u}_n = \frac{1}{2}\widetilde{u}_n - \widetilde{\mathcal{D}}_n\widetilde{u}_n - \widetilde{\mathcal{S}}_n \mathrm{i}k(\lambda\circ\gamma)\widetilde{u}_n + \widetilde{\mathcal{S}}_n \mathrm{i}k\frac{1}{|\gamma'|}P_n'\frac{(\mu\circ\gamma)}{|\gamma'|}P_n'\widetilde{u}_n + \widetilde{\mathcal{S}}_n g_z(\cdot,\widetilde{u}_{n-1};\widetilde{u}_n)\,,$$

where $\widetilde{u}_n = u_n\circ\gamma$, see Section 4.5.

The entries of the matrix representation $\phi(\mathcal{B})$ are then given by

$$\begin{aligned}
\mathrm{Re}\,(B+B_{\#}) = {} & \frac{1}{2}I - \mathrm{Re}\,(\widetilde{\mathcal{D}}_n) + \mathrm{Im}\,(\widetilde{\mathcal{S}}_n)k\mathrm{Re}\,(\lambda) + \mathrm{Re}\,(\widetilde{\mathcal{S}}_n)k\mathrm{Im}\,(\lambda)\\
& - \mathrm{Re}\,(\widetilde{\mathcal{S}}_n)\frac{k}{|\gamma'|}P_n'\frac{\mathrm{Im}\,(\mu\circ\gamma)}{|\gamma'|}P_n' - \mathrm{Im}\,(\widetilde{\mathcal{S}}_n)\frac{k}{|\gamma'|}P_n'\frac{\mathrm{Re}\,(\mu\circ\gamma)}{|\gamma'|}P_n'\\
& + \mathrm{Re}\,(\widetilde{\mathcal{S}}_n)\mathrm{Re}\,(g_z(\cdot,u_{n-1};\mathbb{1})) - \mathrm{Im}\,(\widetilde{\mathcal{S}}_n)\mathrm{Im}\,(g_z(\cdot,u_{n-1};\mathbb{1}))\,,
\end{aligned}$$

$$\begin{aligned}
\mathrm{Im}\,(-B+B_{\#}) = {} & \mathrm{Im}\,(\widetilde{\mathcal{D}}_n) + \mathrm{Re}\,(\widetilde{\mathcal{S}}_n)k\mathrm{Re}\,(\lambda) - \mathrm{Im}\,(\widetilde{\mathcal{S}}_n)k\mathrm{Im}\,(\lambda)\\
& - \mathrm{Re}\,(\widetilde{\mathcal{S}}_n)\frac{k}{|\gamma'|}P_n'\frac{\mathrm{Re}\,(\mu\circ\gamma)}{|\gamma'|}P_n' + \mathrm{Im}\,(\widetilde{\mathcal{S}}_n)\frac{k}{|\gamma'|}P_n'\frac{\mathrm{Im}\,(\mu\circ\gamma)}{|\gamma'|}P_n'\\
& - \mathrm{Re}\,(\widetilde{\mathcal{S}}_n)\mathrm{Im}\,(g_z(\cdot,\xi u_{n-1};\mathbb{1})) - \mathrm{Im}\,(\widetilde{\mathcal{S}}_n)\mathrm{Re}\,(g_z(\cdot,\xi u_{n-1};\mathbb{1}))\,,
\end{aligned}$$

$$\begin{aligned}
\mathrm{Im}\,(B+B_{\#}) = {} & -\mathrm{Im}\,(\widetilde{\mathcal{D}}_n) - \mathrm{Re}\,(\widetilde{\mathcal{S}}_n)k\mathrm{Re}\,(\lambda) + \mathrm{Im}\,(\widetilde{\mathcal{S}}_n)k\mathrm{Im}\,(\lambda)\\
& + \mathrm{Re}\,(\widetilde{\mathcal{S}}_n)\frac{k}{|\gamma'|}P_n'\frac{\mathrm{Re}\,(\mu\circ\gamma)}{|\gamma'|}P_n' - \mathrm{Im}\,(\widetilde{\mathcal{S}}_n)\frac{k}{|\gamma'|}P_n'\frac{\mathrm{Im}\,(\mu\circ\gamma)}{|\gamma'|}P_n'\\
& + \mathrm{Re}\,(\widetilde{\mathcal{S}}_n)\mathrm{Im}\,(g_z(\cdot,u_{n-1};\mathbb{1})) + \mathrm{Im}\,(\widetilde{\mathcal{S}}_n)\mathrm{Re}\,(g_z(\cdot,u_{n-1};\mathbb{1}))\,,
\end{aligned}$$

$$\begin{aligned}
\mathrm{Re}\,(B-B_{\#}) = {} & \frac{1}{2}I - \mathrm{Re}\,(\widetilde{\mathcal{D}}_n) + \mathrm{Im}\,(\widetilde{\mathcal{S}}_n)k\mathrm{Re}\,(\lambda) + \mathrm{Re}\,(\mathcal{S})k\mathrm{Im}\,(\lambda)\\
& - \mathrm{Re}\,(\widetilde{\mathcal{S}}_n)\frac{k}{|\gamma'|}P_n'\frac{\mathrm{Im}\,(\mu\circ\gamma)}{|\gamma'|}P_n' - \mathrm{Im}\,(\widetilde{\mathcal{S}}_n)\frac{k}{|\gamma'|}P_n'\frac{\mathrm{Re}\,(\mu\circ\gamma)}{|\gamma'|}P_n'\\
& + \mathrm{Re}\,(\widetilde{\mathcal{S}}_n)\mathrm{Re}\,(g_z(\cdot,\xi u_{n-1};\mathbb{1})) - \mathrm{Im}\,(\widetilde{\mathcal{S}}_n)\mathrm{Im}\,(g_z(\cdot,\xi u_{n-1};\mathbb{1}))\,.
\end{aligned}$$

By inverting the matrix $\phi(\mathcal{B})$, the real and imaginary parts of the solution $\widetilde{u}_n$ to the integral equation (4.18) can be calculated by

$$\begin{pmatrix} \mathrm{Re}\,(\widetilde{u}_n) \\ \mathrm{Im}\,(\widetilde{u}_n) \end{pmatrix} = (\phi(\mathcal{B}))^{-1} \begin{pmatrix} \mathrm{Re}\,(f \circ \gamma) \\ \mathrm{Im}\,(f \circ \gamma) \end{pmatrix} .$$

APPENDIX C

Representation of $F'[r]$ and $F'[r]^*$ in the Linear Case

To calculate the update of the boundary curve using the regularized Newton method, we need both the Fréchet derivative F' of the far-field operator and its adjoint F'^*. A representation of these operators in the L^2 sense can be determined for the linear case, i.e., for $g \equiv 0$.

The following theorem shows a representation of the far-field pattern u'_∞, which can be derived from the domain derivative u'.

Theorem C.1. *Let u be the solution of the scattering problem (SP) with linear boundary condition, i.e., $g \equiv 0$ and star-shaped scattering object D. The notation $u(\cdot;\theta)$ is intended to indicate the dependence of the solution u of the scattering problem on the incident direction $\theta \in S^1$.*

Then, a representation of the Fréchet derivative of the far-field operator F is given by

$$\begin{aligned} F'[\partial D]h = \frac{\mathrm{e}^{\mathrm{i}\pi/4}}{\sqrt{8\pi k}} \int_{\partial D} h_\nu \Big[& \nabla_\tau u(y;\theta) \cdot \nabla_\tau u(y;-\hat{x}) - k^2 u(y;\theta) u(y,-\hat{x}) \\ & + \mathrm{i}k \left(2\lambda\kappa u(y;\theta) + \lambda \frac{\partial u(y;\theta)}{\partial \nu} + \frac{\partial \lambda}{\partial \nu} u(y;\theta) \right) u(y;-\hat{x}) \\ & + \mathrm{i}k \left(2\mu\kappa + \frac{\partial \mu}{\partial \nu} - 2\mu J_\nu \right) \nabla_\tau u(y;\theta) \cdot \nabla_\tau u(y;-\hat{x}) \\ & + \mathrm{i}k\mu \nabla_\tau \frac{\partial u(y;\theta)}{\partial \nu} \cdot \nabla_\tau u(y;-\hat{x}) \Big] \, \mathrm{d}s_y \, . \end{aligned}$$

This representation is easily obtained by differentiating equation (4.1), inserting the boundary condition (2.11) for $u(\cdot,-\hat{x})$ and applying the second Green's formula, see e.g. [Het99, Corollary 4.25]. Note that the result can be transferred to domains in $\mathbb{R}^3$ by replacing the factor $\gamma_2 = \mathrm{e}^{\mathrm{i}\pi/4}/\sqrt{8\pi k}$ with $\gamma_3 = 1/(4\pi)$.

In addition to the Fréchet derivative of the far-field operator, we require a representation of the associated adjoint operator. In the linear case, such a representation can be determined for star-shaped scattering obstacles.

Theorem C.2. *Let u be the solution of the scattering problem (SP) with linear boundary condition, i.e. $g \equiv 0$ and star-shaped scattering object D.*

Then the adjoint operator to $F'[r]\colon C^k(0,2\pi) \to L^2(S^1)$ is given by

$$\begin{aligned}\overline{(F'[r])^* g(t)} = r(t)\Big[&\nabla_\tau u(y(t);\theta)\cdot\nabla_\tau w(y(t)) - k^2 u(y(t);\theta)w(y(t))\\ &+ \mathrm{i}k\left(2\lambda\kappa u(y(t);\theta) + \lambda\frac{\partial u}{\partial\nu}(y(t);\theta) + \frac{\partial\lambda}{\partial\nu}u(y(t);\theta)\right)w(y(t))\\ &+ \mathrm{i}k\left(2\mu\kappa + \frac{\partial\mu}{\partial\nu} - 2\mu J_\nu\right)\nabla_\tau u(y(t);\theta)\cdot\nabla_\tau w(y(t))\\ &+ \mathrm{i}k\mu\nabla_\tau\frac{\partial u(y(t);\theta)}{\partial\nu}\cdot\nabla_\tau w(y)\Big],\end{aligned}$$

where $w = w^s + w^i$ is defined by the radiating solution w^s of the Helmholtz equation in $\mathbb{R}^2\backslash\overline{D}$ and $w^s = -w^i$ on ∂D with the Herglotz wave function

$$w^i(y) = \frac{\mathrm{e}^{\mathrm{i}\pi/4}}{\sqrt{8\pi k}}\int_{S^1}\overline{g(\hat{x})}e^{-\mathrm{i}ky\cdot\hat{x}}\,\mathrm{d}s_{\hat{x}}, \quad y\in\mathbb{R}^2.$$

This result is obtained by differentiating equation (4.1), inserting the boundary condition (2.11) for $u(\cdot,-\hat{x})$ with $g\equiv 0$, and applying the second Green's formula in $\mathbb{R}^2\backslash\overline{D}$.

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Notation

Basic notation

$\mathbb{N}_0$	natural numbers including zero	
$\mathbb{R}^d$	d-dimensional real Euclidean space	
$\mathbb{C}^d$	d-dimensional complex Euclidean space	
$x \cdot y$	inner product of $x, y \in \mathbb{R}^d$	
$x \times y$	vector product of $x, y \in \mathbb{R}^d$	
$\lvert x \rvert$	Euclidean norm of $x \in \mathbb{R}^d$	
Ω	open domain	
$\partial\Omega$	boundary of Ω	
$\overline{\Omega}$	closure of Ω	
$B_R(0)$	ball of radius R in $\mathbb{R}^d$ centered at the origin	15
$B'_{r_j}(0)$	ball of radius r_j in $\mathbb{R}^{d-1}$ centered at the origin	9
S^{d-1}	unit sphere in $\mathbb{R}^d$	7
$\hat{x}$	direction $x/\lvert x \rvert \in S^{d-1}$	11
j	multi-index of order $\lvert j \rvert = j_1 + \ldots + j_d$	7
∂^j	differential operator	7
ν	unit outward normal on $\partial\Omega$	9
$\partial u/\partial \nu$	normal derivative of u on $\partial\Omega$	10
h_ν	normal component of a vector field h	38
h_τ	tangential component of a vector field h	38
D	scattering object, bounded domain in $\mathbb{R}^d$	11
D_h	domain D perturbed by a vector field h	37
D_{pc}	perfectly conductive scattering object	13
$\mathcal{U}_\delta$	thin layer of thickness δ	13
Ω_R	bounded domain $B_R(0)\backslash\overline{D}$	15
$\Omega_{R,h}$	bounded domain $B_R(0)\backslash\overline{D}_h$	38

κ	mean curvature of ∂D	14
$\mathrm{Det}(\varphi)$	Jacobian with respect to ∂D	39
p	pressure	10
c_0	speed of sound	10
k	wave number	11
θ	propagation direction	11
ρ	density	11
ω	angular frequency	11
ϵ_0	electric permittivity in free space	13
μ_0	magnetic permeability in free space	13
ϵ_1	electric permittivity in the thin layer	13
μ_1	magnetic permeability in the thin layer	13
H	magnetic field	13
$\mathbb{1}$	vector of ones of appropriate size	62

FUNCTION SPACES

$C^k(\Omega)$	k times continuously differentiable functions on Ω, $k \in \mathbb{N}_0 \cup \{\infty\}$	7
$C_c^k(\Omega)$	C^k functions with compact support on Ω, $k \in \mathbb{N}_0 \cup \{\infty\}$	7
$C^1(\overline{\Omega})$	functions in $C^1(\Omega)$ whose derivatives have continuous extensions to $\overline{\Omega}$	9
$C^{k,\alpha}(\Omega)$	Hölder space with exponent α on Ω, $0 < \alpha \leq 1$, $k \in \mathbb{N}_0$	7
$C_p^2(0, 2\pi)$	twice continuously differentiable 2π-periodic functions	57
$C(\partial\Omega)$	continuous functions on $\partial\Omega$	9
$C^1(\partial\Omega)$	continuously differentiable functions on $\partial\Omega$	9
$C_t^1(\partial\Omega)$	tangential vector fields in $C^1(\partial\Omega)$	9
$L^p(\Omega)$	Lebesgue space on Ω, $1 \leq p \leq \infty$	8
$L^p_{\mathrm{loc}}(\Omega)$	local Lebesgue space on Ω, $1 \leq p \leq \infty$	8
$L^2(\partial\Omega)$	Lebesgue space on $\partial\Omega$, $p = 2$	9
$H^k(\Omega)$	Sobolev space on $\partial\Omega$, $k \in \mathbb{N}$	8
$H^k_{\mathrm{loc}}(\Omega)$	local Sobolev space on $\partial\Omega$, $k \in \mathbb{N}$	8
$H^s(\Omega)$	Sobolev space on Ω, $s \geq 0$	8
$H_0^1(\Omega)$	closure of $C_c^\infty(\Omega)$ in $H^1(\Omega)$	10

H_D	functions in $H^1(\Omega)$ that solve the variational Helmholtz equation	10
$H_{\mathrm{per}}^{-\frac{1}{2}+s}[0,2\pi]$	periodic Sobolev space of order $-1/2+s$ for $s \in [-1,1]$	60
$H^{\frac{1}{2}}(\partial\Omega)$	trace space, range of γ_0	9
$H^{-\frac{1}{2}}(\partial\Omega)$	dual space of $H^{\frac{1}{2}}(\partial\Omega)$	10
$H^s(\partial\Omega)$	Sobolev space on $\partial\Omega$, $s > 1/2$	10
V_R	functions in $H^1(\Omega)$ with boundary values in $H^1(\partial\Omega)$	15
$V_{R,h}$	function in V_R with respect to the perturbed domain Ω_h	38

FUNCTIONS

$\operatorname{supp} u$	support of the function u	7
λ, μ	impedance functions	15
$g(\cdot, u)$	nonlinear function with respect to u	15
$g_z(x, z; w)$	differentiation of g with respect to the second component	19
Φ	fundamental solution to the Helmholtz equation	21, 25
SL	single-layer potential	25
DL	double-layer potential	25
$H_0^{(1)}$	Hankel function of first kind of order zero	25, 60
$H_1^{(1)}$	Hankel function of first kind of order one	60

OPERATORS

L^*	adjoint operator of the operator L	17
$\mathcal{R}(I+L)$	range of the operator $I+L$	17
$\mathcal{N}(I+L^*)$	null space of the operator $I+L^*$	18
Δ	Laplace operator	10
div	divergence of a vector field	12
curl	rotation of a vector field	51
∇_τ	surface gradient	12
Div	surface divergence	12
γ_0	trace operator	9
γ_0^{ext}	exterior trace operator	32

γ_1	normal derivative trace operator	10
$\mathcal{S}$	single-layer operator	21, 26
$\mathcal{D}$	double-layer operator	21, 26
$\mathcal{D}'$	adjoint double-layer operator	26
$\widetilde{\mathcal{S}}$	parameterized single-layer operator	60
$\widetilde{\mathcal{D}}$	parameterized double-layer operator	67
$\widetilde{\mathcal{D}}'$	parameterized adjoint double-layer operator	60
Λ	Dirichlet-to-Neumann operator	16
G	Nemytskii operator, induced by g	16
R_l	linear part of the operator R	18
R_n	nonlinear part of the operator R	18
F	domain-to-far-field operator	56
$\mathbb{F}$	all-at-once system of model and observation equation	69

Index