

Theoretical aspects of the application of convolution quadrature to scattering of acoustic waves

Antonio R. Laliena · Francisco-Javier Sayas

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Abstract In this paper we address several theoretical questions related to the numerical approximation of the scattering of acoustic waves in two or three dimensions by penetrable non-homogeneous obstacles using convolution quadrature (CQ) techniques for the time variable and coupled boundary element method/finite element method for the space variable. The applicability of CQ to waves requires polynomial type bounds for operators related to the operator $\Delta - s^2$ in the right half complex plane. We propose a new systematic way of dealing with this problem, both at the continuous and semidiscrete-in-space cases. We apply the technique to three different situations: scattering by a group of sound-soft and -hard obstacles, by homogeneous and non-homogeneous obstacles.

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1 Introduction

Physical problem. In this paper we address several theoretical questions related to the numerical approximation of the scattering of acoustic waves in two or three dimensions by penetrable non-homogeneous obstacles using convolution quadrature (CQ)

A. R. Laliena
Dep. Matemáticas, EUPLA, Universidad de Zaragoza, 50100 La Almunia, Spain
e-mail: antonio.laliena@eupla.unizar.es

F.-J. Sayas (✉)
Dep. Matemática Aplicada, CPS, Universidad de Zaragoza, 50018 Zaragoza, Spain
e-mail: jsayas@unizar.es

F.-J. Sayas
School of Mathematics, University of Minnesota, 206 Church St. SE,
Minneapolis, MN 55455, USA

techniques for the time variable and coupled boundary element method/finite element method (BEM–FEM) for the space variable.

We begin by setting precisely the problem. Let Ω_- be a bounded open set in \mathbb{R}^d ($d = 2$ or 3), with Lipschitz boundary and connected complement. The complement is denoted Ω_+ and the common interface, Γ . The set (the obstacle) can be non-connected but we preclude the possibility of it having inclusions. Given an incident wave field in free space u_{ind} we try to compute the scattering produced by the presence of the obstacle in the wave field: for all $t > 0$

$$\begin{cases} \Delta u_{\text{scat}} - u_{\text{scat},tt} = 0, & \text{in } \Omega_+, \\ u_{\text{scat}} + u_{\text{inc}} = u_{\text{in}}, & \text{on } \Gamma, \\ \partial_\nu u_{\text{scat}} + \partial_\nu u_{\text{inc}} = \kappa_0 \partial_\nu u_{\text{in}}, & \text{on } \Gamma, \\ \nabla \cdot (\kappa_0 \nabla u_{\text{in}}) - \kappa_1 u_{\text{in},tt} = 0, & \text{in } \Omega_-. \end{cases}$$

We assume that both u_{inc} and its time derivative vanish in a region that strictly contains $\overline{\Omega_-}$ at time zero, so the physical placement of the obstacle is feasible. Therefore the scattered field u_{scat} and the total field inside the obstacle, u_{in} , satisfy:

$$u_{\text{scat}}(\cdot, 0) \equiv u_{\text{scat},t}(\cdot, 0) \equiv 0, \quad u_{\text{in}}(\cdot, 0) \equiv u_{\text{in},t}(\cdot, 0) \equiv 0.$$

Because of the finite speed of propagation of solutions of the wave equation we have the radiation condition: for all t there exists $R(t) > 0$ such that $u_{\text{scat}}(\mathbf{x}, t) \equiv 0$, if $|\mathbf{x}| \geq R(t)$. This condition is never set explicitly since it comes together with the causality of the wave equation and the fact that the traces left by the incident wave on the interface form a set of compactly supported data. The parameters for the interior domain can depend on the space variable but not on time. In terms of physical magnitudes, κ_0 and κ_1 are, respectively, defined to be $1/\rho$ and $1/(c^2\rho)$, where ρ is the density in the equilibrium state and c is the speed of propagation of sound. Both parameters have been set equal to one in the exterior domain. We will consider three situations: (a) the general case with non-constant coefficients, which will need a boundary-field (BEM–FEM) formulation, (b) the case with constant coefficients, which can be formulated only with integral equations, (c) the purely exterior case, when the obstacles are either sound-soft or sound-hard, so that the pressure u_{in} is not computed inside the obstacles and we choose one of the Dirichlet or Neumann conditions setting the interior value to zero. As we will see, the combination of soft and hard obstacles will arise very naturally in our formulation and we will be able to deal with it as a particular case of exterior problems with mixed boundary values.

Note that unlike in the time-harmonic case (corresponding to a time-harmonic incident wave after enough time has gone by so that the resulting scattered wave can be effectively considered time-harmonic itself), the decomposition of the total wave field as the sum of incident and scattered fields leads to an apparent paradox. Indeed, even if the incident wave hits the obstacle on one side and the wave speed of propagation is slower inside the obstacle than in the surrounding fluid, the scattered field produced by the object in the opposite extreme begins to appear before the real wave reaches that part of the obstacle, as if the wave had crossed it at the exterior velocity or surrounded it faster than possible. This is just a false paradox produced by the fact that

the incident wave is a wave in free space. As such, it reaches each point of the obstacle as if this one were not present. Therefore, at the beginning scattering is just the needed compensation for the fact that the wave has not reached still a certain region.

Integral representation. In the three-dimensional case, the exterior scattered field can be represented using Kirchhoff's formula, an expression that uses both the single- and double-layer retarded acoustic potentials. A similar formula exists in the two-dimensional case, with the well-known difference of a memory effect in the propagation of waves. Imposing the coupled transmission conditions of the solution using a weak formulation inside the obstacle and the integral representation outside leads to one of several possible coupled boundary-field formulations.

The coupled problem can be understood as a convolution operator equation in time. This can be easily done as follows. First we take the Laplace transform of the original problem. Thanks to the vanishing initial conditions, the equations in the Laplace domain (henceforth referred to as the frequency domain) become

$$\Delta u_{\text{scat}} - s^2 u_{\text{scat}} = 0, \quad \nabla \cdot (\kappa_0 \nabla u_{\text{in}}) - s^2 \kappa_1 u_{\text{in}} = 0,$$

where we have kept the same name for the unknowns that depend now on $\mathbf{x} \in \Omega_{\pm}$ and s in the complex plane. Then, we use Green's Third Theorem (Formula or Identity) to give a representation of the exterior solution and obtain a coupled boundary-field formulation for each of these steady-state problems. The fact that multiplication (application of operators to functions) in the frequency domain corresponds to convolution in time can be used to show that both the operator equation and its inverse are in fact causal convolution equations, i.e., convolution equations with all the elements (operators, data, unknowns) beginning at time zero. A very precise description of how Kirchhoff's formula can be read as a convolution formula for certain vector-valued distributions is given in [24].

Historical notes on convolution quadrature. The fact that we obtain a convolution equation suggests the possibility of using CQ methods for the time variable together with a natural BEM–FEM discretization in space (which is the most reasonable approach to approximate the coupled problem in the frequency domain). By extending classical ideas of discrete operational calculus, Christian Lubich introduced CQ in the late eighties [25, 26]. For the analysis of Runge–Kutta methods for parabolic equations, the CQ technique was extended to a new class of methods based on RK schemes [29]. The analysis of this class of methods has recently been extended in [5]. The relevant paper for our purposes is [27], where the first example of a CQ method for a retarded integral equation is proposed and analyzed. There was a precedent of using CQ for boundary integral equations in [30], for the single-layer potential of the heat equation. More recently, Rothe's method for the heat equation was successfully analyzed in [7] by interpreting it as a CQ scheme (Rothe's method for the wave equation as explained in [31] admits the same treatment). Some unexpected relations of CQ with algorithms of digital signal processing are mentioned in [33]. Recent work both at the theoretical level [28] and on fast implementation techniques [35] applies exclusively to equations with parabolic character, where the domain of the Laplace

transform crosses the imaginary axis in the form of the complementary of a sector around the negative real axis, or equivalently, the corresponding time operator (the semigroup in the parabolic equation) admits an holomorphic extension. This is not the case for any of the problems of our interest. A short exposition of the simplest CQ method is given in Appendix 1.

Although we will eventually give some expressions for the time-domain potentials *we will write all the equations in the frequency domain*. It has to be understood however, that *this method works in the time domain*, so data are employed causally, as they arrive to the interface, and solutions are computed in a time-stepping fashion. The fact that we will be using the operators in the frequency domain (which is a requisite of CQ) does not mean that we are solving in that domain and then inverting the Laplace transform. This is a valid strategy for many problems of parabolic type (see [20,38]) but does not work for wave propagation. In addition to that, such approach would have the disadvantage of requiring knowledge of the Laplace transform of the data instead of using time steps.

What we do in this paper. Here we intend to set clearly what is needed for the application of a fully discrete (space–time) CQ–BEM–FEM to our problem. We want to remark right at this point that we are still at a certain distance of being able to offer a full effective numerical simulation of the problem and that some of the estimates could be non-optimal. Note that application of CQ techniques to wave propagation has been mainly done in the area of purely exterior problems, be it in the original paper [27], in recent work [17,21] and in many applications to interesting problems of elastic wave propagation (including viscoelastic and poroelastic waves) [36].

In Sect. 2, we will describe precisely the class of functions in the transformed frequency domain that we will be dealing with. In Sect. 3 we will introduce all the integral potentials and operators that will be used in the remainder of the paper. We will also give a statement concerning how these operators belong to the abstract classes of the preceding section, even though we will postpone the proofs to Appendix 2. In Sect. 4 we will finally give the first example of how our technique works. First we will state a general lemma about a class of variational problems depending on the complex parameter s . Instead of going directly to one of the three situations under consideration, we will first illustrate the novel technique of proof by showing how it works with a simple example related to a symmetric boundary integral representation of the exterior Steklov–Poincaré operator and its Galerkin discretization. As far as we have been able to gather from existing literature, our approach is original: it consists of understanding boundary integral systems, both at the discrete and continuous level, as non-standard transmission problems. The gist of the method will consist of four steps: (1) find the non-standard transmission problem that is equivalent to the boundary integral system; (2) find the equivalent weak formulation of this problem; (3) prove well-posedness of the variational problem and bounds depending on s following the general lemma; (4) go back to the original problem and gather the information given by the chain of equivalences.

The following four sections cover the three physical settings. Section 5 deals with exterior problems where sound-hard and sound-soft scatterers coexist. We will see how the four-step technique works simultaneously for the discrete and the continuous

problem. In Sect. 6 we study the case of non-homogeneous penetrable obstacles. The space discretization will be done by using an abstract Finite Element space for the interior variable and two Boundary Element spaces for unknowns on the interface. The coupling procedure will be the symmetric coupling with two equations and three unknowns as in [6]. The symmetric coupling procedure of [8] or [19] is studied in Sect. 7 in two different implementable formulations. This coupling method uses essentially the trace space of the finite element space as one of the boundary element spaces, but is not equivalent to the three-space coupling. Finally in Sect. 8 we deal with homogeneous penetrable obstacles and use the symmetric coupling of Costabel and Stephan [11] to write everything in terms of integral operators.

In many cases, data appear under the action of time operators. In those cases, we understand that the corresponding time-convolutions have also to be discretized and we have accordingly analyzed this discretization. We have also covered the possibility of the space discretization of data before plugging them into integral operators. This is a very common way of treating data in the engineering literature of boundary integral methods and has the advantage of making the algorithms closer to the implementation level. We have also taken into account the fact that what is of interest for us are not the quantities on the boundary but the pressure field that requires an integral postprocessing. Everything that we do here can be extended almost verbatim to the case of elastic waves in two and three dimensions.

Still to be done. Because we want to emphasize the novel aspects of our approach with several situations of interest, we only study the behavior of all the systems with respect to the variable in the frequency domain. This behavior conditions on the applicability of CQ and on the regularity of the solution to retain the full order of convergence of the method. We do this only in the natural Sobolev norms (H^1 in the domain, $H^{1/2}$ for traces, $H^{-1/2}$ for normal derivatives). At this point we can apply the theory of Lubich [27]. To obtain a full space-and-time estimate with precise conditions on the regularity of the solution, there is still some work to be done concerning bounds for the solution. This will require to plunge back into results as the ones in Appendix 2 and to revert many estimates in the frequency domain to the adequate norms of functions depending on the time and space variables. This is the aim of future work. We believe that our objectives here are clearly set and have been fully attained. The complete analysis for all the situations will require some additional pages of estimates that we prefer not to give here, not only to help readability (the article is long enough as it is and has its share of technicalities, although we do not use very sophisticated results) but also to emphasize the novelties.

Other approaches to time-domain integral equations. The CQ approach is not the only possible for exterior problems and is not even the most commonly used. Many authors in the French school of Numerical Analysis have studied the numerical approximations of retarded integral equations for scattering problems of acoustic, elastic and electromagnetic waves, almost exclusively in three dimensions. The papers [2,3] study the numerical approximation of the single- and double-layer retarded acoustic potentials in three dimensions. Extensions of these results are many (see [1,4,16] and the references in the review [15]), all of them dealing with Galerkin methods. For the

collocation method applied to the single-layer retarded potential, see [14]. The main advantage of working directly with these equations relies on the locality in time (which is lost with CQ, because of the regularization imposed by its approximation through the Laplace transform). Nevertheless, practical implementation becomes a very delicate question, for the extreme complexity of the integration domains in time-and-space. This is even harder in the case of elastic waves and there is no hope for visco-elastic or poro-elastic waves, since the time-domain fundamental solutions are not known. Also in the two-dimensional case the advantage of working directly with the time-domain operators is not so relevant, because of the natural memory terms. The advantage of CQ is also seen in other equations with memory [12], often modeled with fractional order derivatives. In addition to [15] an extensive and recent review of time-domain integral equations is [10].

Sobolev space prerequisites. Extensive use will be made of the most basic Sobolev spaces on domains and closed boundaries. The letter γ will always be used for the trace operator. Super/subscripts \pm will be used to clarify if these traces are taken from outside or inside the boundary. The weak normal derivative, with the normal vector pointing always outwards (inwards from the point of view of the exterior domain) will be denoted ∂_ν or ∂_ν^\pm . A good reference for Sobolev spaces on Lipschitz domains, as will be used here, is [32], which has also the advantage of including detailed proofs of the general results about boundary integral operators for elliptic problems that we will make use of. All boundaries are considered to be Lipschitz. There is no reason to need them connected, but we will exclude the case when one of the boundaries encloses another, that is, it will be generally assumed that the exterior domain is connected, even if the interior one is composed of more than one connected component. The square bracket will be used for jumps across the boundaries, and thus

$$[\gamma u] = \gamma^- u - \gamma^+ u, \quad [\partial_\nu u] = \partial_\nu^- u - \partial_\nu^+ u.$$

The space of infinitely often differentiable functions with compact support in an open set \mathcal{O} will be denoted $\mathcal{D}(\mathcal{O})$.

Notational foreword. Because there will be many operators and spaces involved in the sequel, we will keep a very strict convention for character types. In formulas, capital Roman letters (F, V, \dots) will be used for operators, very often depending on a complex parameter, in which case the dependence will be written explicitly $F(s)$, whereas the action on an element of the origin space will be written in multiplicative form $F(s)u$. Boldface capitals (such as \mathbf{H}) will be used for matrices of operators.

Spaces will be always denoted with mathematical capitals (H, X, \dots) and the subscript h will be used to make discretization in the space variables explicit. Very often we will have a subspace $X \subset H$. Then we will denote by $X : X \rightarrow H$ the canonical inclusion of X into H and by $X' : H' \rightarrow X'$ its transpose, which simply restricts the action of an element of H' to the elements of X (the prime index is used to denote the dual space). The polar set (or annihilator) of X will be denoted $X^\circ := \{f \in H' \mid \langle f, x \rangle = 0, \forall x \in X\}$.

Duality is going to be an issue all along this paper. To avoid the excessive weight of multiple subscripts hanging from all the duality brackets, we will simply use the angled bracket $\langle f, x \rangle$ for the action of $f \in H'$ on $x \in H$, whatever H is. The bracket is linear (not conjugate linear) in both components. There is not going to be ambiguity on which are the primal and dual spaces in each of the expressions.

The spaces $H^{\pm 1/2}(\Gamma)$ are dual of each other as an extension of the *real* inner product in $L^2(\Gamma)$. When used on elements of these spaces, it has to be understood that *even with complex valued functions*

$$\langle f, g \rangle \text{ extends } \int_{\Gamma} fg \text{ for } f \in H^{-1/2}(\Gamma) \text{ and } g \in H^{1/2}(\Gamma),$$

always in this order and with no conjugation. This will be the only exception where the dual space can be in the second component, namely, when $H^{1/2}(\Gamma)$ is considered as the dual space of $H^{-1/2}(\Gamma)$.

2 Abstract concepts

Consider two complex Hilbert spaces X and Y and let $\mathcal{L}(X, Y)$ be the space of bounded linear operators from X to Y . We set

$$\mathbb{C}_+ := \{s \in \mathbb{C} \mid \operatorname{Re} s > 0\}.$$

For a given $\mu \in \mathbb{R}$, the elements of the class $\mathcal{A}(\mu, X, Y)$ are the analytic functions $F : \mathbb{C}_+ \rightarrow \mathcal{L}(X, Y)$ for which there exists a real number μ such that for all $\sigma > 0$ there is $C_0 = C_0(\sigma)$ such that

$$\|F(s)\| \leq C_0 |s|^\mu, \quad \forall s \text{ s.t. } \operatorname{Re} s > \sigma.$$

Equivalently we can write that there exists a non-increasing function $C_0 : (0, \infty) \rightarrow (0, \infty)$ such that

$$\|F(s)\| \leq C_0(\operatorname{Re} s) |s|^\mu, \quad \forall s \in \mathbb{C}_+.$$

It is clear that $\mathcal{A}(\mu, X, Y)$ is a complex vector space and that these classes are ordered by the parameter μ :

$$\mathcal{A}(\mu, X, Y) \subset \mathcal{A}(\mu + \varepsilon, X, Y), \quad \forall \varepsilon > 0.$$

If X, Y and Z are Hilbert spaces it is easy to see that

$$F \in \mathcal{A}(\mu_1, Y, Z), \quad G \in \mathcal{A}(\mu_2, X, Y), \quad \implies \quad FG \in \mathcal{A}(\mu_1 + \mu_2, X, Z). \quad (1)$$

In any case, let us emphasize that this composition rule gives only an upper bound of μ (which is a parameter reflecting lack of regularity) and that, because of cancelations,

we will find very often that composition decreases the value of this parameter. In this respect one has to abandon the false intuition of dealing with operators in this family as ‘monomials’ that always increase degree by multiplication.

The following two results relate the functions of the preceding classes to be Laplace transforms of some functions or tempered distributions. Their proofs follow classical arguments of distribution theory, complex analysis and the formula for the inverse of the Laplace transform. Proofs of very similar results (the functional classes are not exactly the same) can be found in any text that includes the distributional approach to the Laplace transform, such as [37].

Theorem 1 *Let $F \in \mathcal{A}(\mu, X, Y)$ with $\mu < -1$. Then there exists a continuous function $f : \mathbb{R} \rightarrow \mathcal{L}(X, Y)$ such that $\text{supp } f \subseteq [0, \infty)$ and such that its Laplace transform, defined in \mathbb{C}_+ , is F . If $\mu < -k - 1$ with k positive integer, then $f \in \mathcal{C}^k(\mathbb{R}, \mathcal{L}(X, Y))$.*

Implicit in the fact that there exists the Laplace transform of f in \mathbb{C}_+ is the fact that $\exp(-\sigma \cdot) f$ is a tempered distribution with values in $\mathcal{L}(X, Y)$ for all $\sigma > 0$, as this allows us to define the Laplace transform. In fact we can prove that

$$\|f(t)\| \leq \exp(\sigma t)C(\sigma, F), \quad \forall \sigma > 0, \quad \forall t,$$

which ensures that $\exp(-\sigma \cdot) f$ is tempered.

Theorem 2 *Let $F \in \mathcal{A}(\mu, X, Y)$ with $\mu \geq -1$. Take k such that $1 + \mu < k \leq 2 + \mu$. Then there exists $g \in \mathcal{C}(\mathbb{R}, \mathcal{L}(X, Y))$ such that $\text{supp } g \subseteq [0, \infty)$ and F is the Laplace transform of $g^{(k)}$ in \mathbb{C}_+ , where the derivative is understood in the sense of distributions in \mathbb{R} .*

Constant operators $F(s) \equiv F_0$ belong to $\mathcal{A}(0, X, Y)$. They correspond in the time domain to impulses at $t = 0$, i.e., distributions of the form $\delta_0 \otimes F_0$.

We will consider another class of operators. For these ones we need that the Hilbert spaces involved admit a conjugation operator, such as in the case when they are complexifications of real Hilbert spaces. In this case, the parameters are $\mu \in \mathbb{R}$ and a function $\theta : \mathbb{C}_+ \rightarrow \mathbb{R}$. We write that $F \in \mathcal{E}(\mu, \theta, X)$ when $F : \mathbb{C}_+ \rightarrow \mathcal{L}(X, X')$ is analytic and there exists a non-decreasing function $c : (0, \infty) \rightarrow (0, \infty)$ such that

$$\text{Re} \left(e^{i\theta(s)} \langle F(s)\psi, \bar{\psi} \rangle \right) \geq \frac{c(\text{Re } s)}{|s|^\mu} \|\psi\|^2, \quad \forall \psi \in X, \quad \forall s \in \mathbb{C}_+. \tag{2}$$

The classes $\mathcal{E}(\mu, \theta, X)$ are vector spaces and they are ordered in μ

$$\mathcal{E}(\mu, \theta, X) \subset \mathcal{E}(\mu + \varepsilon, \theta, X), \quad \varepsilon > 0.$$

Proposition 3 *If $F \in \mathcal{E}(\mu, \theta, X)$, then $F^{-1} \in \mathcal{A}(\mu, X', X)$.*

Proof The inequality (2) implies that $F(s)$ is invertible for all $s \in \mathbb{C}_+$. If $F : \mathbb{C}_+ \rightarrow \mathcal{L}(X, Y)$ is analytic and $(F(s))^{-1}$ exists for all $s \in \mathbb{C}_+$, then F^{-1} is analytic as a function with values in $\mathcal{L}(Y, X)$. The ellipticity condition permits to prove that $\|F(s)^{-1}\| \leq \frac{1}{c(\text{Re } s)} |s|^\mu$, which shows that F^{-1} is in the corresponding class. \square

Let now X_h and Y_h be two sequences of spaces and assume that $F_h \in \mathcal{A}(\mu, X_h, Y_h)$. We write that

$$F_h \in \mathcal{A}^{\text{unif}}(\mu, X_h, Y_h)$$

when the functions C_0 do not depend on h .

Proposition 4 (Galerkin projections) *Let $F \in \mathcal{A}(\mu, X, Y')$ and consider two sequences of subspaces*

$$X_h \subset X, \quad Y_h \subset Y$$

and the operators $F_h : \mathbb{C}_+ \rightarrow \mathcal{L}(X_h, Y'_h)$ defined by

$$F_h(s)x_h := \langle F(s)x_h, \cdot \rangle : Y_h \rightarrow \mathbb{C}.$$

Then $F_h \in \mathcal{A}^{\text{unif}}(\mu, X_h, Y'_h)$. If, on the other hand, $F \in \mathcal{E}(\mu, \theta, X)$, then $F_h^{-1} \in \mathcal{A}^{\text{unif}}(\mu, X'_h, X_h)$.

3 Bounds in the resolvent set

We first recall the fundamental solution for the operator $\Delta - s^2$ in two and three dimensions:

$$\Phi(\mathbf{x}, \mathbf{y}, s) := \begin{cases} \frac{i}{4} H_0^{(1)}(is|\mathbf{x} - \mathbf{y}|), & \text{when } d = 2, \\ \frac{e^{-s|\mathbf{x} - \mathbf{y}|}}{4\pi|\mathbf{x} - \mathbf{y}|}, & \text{when } d = 3. \end{cases}$$

Here $H_0^{(1)}$ is the Hankel function of the first kind and order zero. We will consider the layer potentials and integral operators associated to this operator for $s \in \mathbb{C}_+$. Note that with s^2 we are covering $\mathbb{C} \setminus (-\infty, 0]$. Given $\lambda \in H^{-1/2}(\Gamma)$ and $\phi \in H^{1/2}(\Gamma)$ we can define the single- and double-layer potentials with the expressions, valid as dualities on Γ for arbitrary $\mathbf{x} \in \mathbb{R}^d \setminus \Gamma$:

$$\begin{aligned} (\mathbf{S}(s)\lambda)(\mathbf{x}) &:= \int_{\Gamma} \Phi(\mathbf{x}, \mathbf{y}, s) \lambda(\mathbf{y}) \, d\Gamma(\mathbf{y}), \\ (\mathbf{D}(s)\phi)(\mathbf{x}) &:= \int_{\Gamma} \partial_{\nu(\mathbf{y})} \Phi(\mathbf{x}, \mathbf{y}, s) \phi(\mathbf{y}) \, d\Gamma(\mathbf{y}). \end{aligned}$$

The four operators that participate in Calderón’s projector are extensions of the following integral expressions, all of them defining functions on Γ :

$$\begin{aligned}
 V(s)\lambda &:= \int_{\Gamma} \Phi(\cdot, \mathbf{y}, s) \lambda(\mathbf{y}) \, d\Gamma(\mathbf{y}), \\
 K^t(s)\lambda &:= \int_{\Gamma} \partial_{v(\cdot)} \Phi(\cdot, \mathbf{y}, s) \lambda(\mathbf{y}) \, d\Gamma(\mathbf{y}), \\
 K(s)\phi &:= \int_{\Gamma} \partial_{v(\mathbf{y})} \Phi(\cdot, \mathbf{y}, s) \phi(\mathbf{y}) \, d\Gamma(\mathbf{y}), \\
 W(s)\phi &:= -\partial_v \int_{\Gamma} \partial_{v(\mathbf{y})} \Phi(\cdot, \mathbf{y}, s) \phi(\mathbf{y}) \, d\Gamma(\mathbf{y}).
 \end{aligned}$$

With $DtN^{\pm}(s)$, $NtD^{\pm}(s)$ we, respectively, denote the Dirichlet-to-Neumann and Neumann-to-Dirichlet operators for the equation $\Delta u - s^2 u = 0$ in Ω_{\pm} . If $\Delta u - s^2 u = 0$ in $\mathbb{R}^d \setminus \Gamma$ and we denote $[\gamma u] = \gamma^- u - \gamma^+ u$ and $[\partial_v u] = \partial_v^- u - \partial_v^+ u$, then Green’s Third Theorem represents u in potential form

$$u = S(s)[\partial_v u] - D(s)[\gamma u]. \tag{3}$$

A collection of useful formulas related to these operators and potentials is given in Appendix 2 for easy reference. Proofs of these results follow from [9] and can be found in [32] in full generality for Lipschitz domains in any dimension.

Let us briefly recall what some of these operators look like in the time-domain. In three dimensions, the potential $S(s)$ and its trace $V(s)$ correspond in the time domain to the single-layer retarded potential

$$\int_{\Gamma} \frac{\lambda(\mathbf{y}, t - |\mathbf{x} - \mathbf{y}|)}{4\pi |\mathbf{x} - \mathbf{y}|} \, d\Gamma(\mathbf{y}).$$

The potential $D(s)$ corresponds to the double-layer retarded potential

$$\int_{\Gamma} \partial_{v(\mathbf{y})} \left(\frac{\phi(\mathbf{z}, t - |\mathbf{x} - \mathbf{y}|)}{4\pi |\mathbf{x} - \mathbf{y}|} \right) \Big|_{\mathbf{z}=\mathbf{y}} \, d\Gamma(\mathbf{y}),$$

that, as can be seen by formally computing the normal derivative, includes a time derivative of the density ϕ .

Green’s Third Theorem (3) is the frequency domain version of the well-known Kirchhoff formula for solutions of the unforced wave equation in the space. A detailed and precise description of these time convolution operators with very mild regularity assumptions in time and space is given in [24].

In the three-dimensional space, Huygens principle holds and potentials have no memory. However, two-dimensional waves have memory in addition to the delay due to the finite speed of propagation. For instance, the single-layer potential can be formally written as

$$\int_{\Gamma} \left(\int_{|\mathbf{x}-\mathbf{y}|}^t \frac{\psi(\mathbf{y}, t-\tau)}{2\pi\sqrt{\tau^2-|\mathbf{x}-\mathbf{y}|^2}} d\tau \right) d\Gamma(\mathbf{y})$$

$$= \int_{\Gamma} \left(\int_0^{t-|\mathbf{x}-\mathbf{y}|} \frac{\psi(\mathbf{y}, \tau)}{2\pi\sqrt{(\tau-t)^2-|\mathbf{x}-\mathbf{y}|^2}} d\tau \right) d\Gamma(\mathbf{y}).$$

(in both expressions we implicitly assume that $\psi(\cdot, t) \equiv 0$ for $t < 0$). Note however, that these time-domain expressions of the operators are never used in CQ discretizations.

Next, let us briefly discuss a couple of details it is important to be extremely careful about. If we use the complex adjoints, then

$$V^*(s) = V(\bar{s}), \quad W^*(s) = W(\bar{s}), \quad K^*(s) = K^t(\bar{s}).$$

This fact affects the analysis more than expected, since some matrices of operators that we will obtain will be symmetric but not self-adjoint and many of the cancelations that one is used to have when dealing with the Helmholtz equation will not be valid here. Recall the well-known fact that if F is holomorphic then $F(\bar{s})$ is not, unless F is constant. Therefore, modifying the equations with the use of adjoints is not a valid option since we leave the realm of analytic functions, which is a key for applying the results on CQ. On the other hand, we have the symmetry property

$$V^t(s) = V(s), \quad W^t(s) = W(s). \tag{4}$$

The main result of this section, which we will not formulate as a theorem, is contained in Tables 1 and 2. Detailed proofs of these results are given in Appendix 2. Some of them had already appeared in the literature of time-domain integral equations.

Table 1 Classes corresponding to operators in the resolvent set of the Laplacian

F	X	Y	μ
S	$H^{-1/2}(\Gamma)$	$H^1(\mathbb{R}^d)$	1
D	$H^{1/2}(\Gamma)$	$H^1(\mathbb{R}^d \setminus \Gamma)$	3/2
V	$H^{-1/2}(\Gamma)$	$H^{1/2}(\Gamma)$	1
W	$H^{1/2}(\Gamma)$	$H^{-1/2}(\Gamma)$	2
K	$H^{1/2}(\Gamma)$	$H^{1/2}(\Gamma)$	3/2
K^t	$H^{-1/2}(\Gamma)$	$H^{-1/2}(\Gamma)$	3/2
DtN^\pm	$H^{1/2}(\Gamma)$	$H^{-1/2}(\Gamma)$	2
NtD^\pm	$H^{-1/2}(\Gamma)$	$H^{1/2}(\Gamma)$	1

The assertion for each row is given by the first line, a prototype denoting $F \in \mathcal{A}(\mu, X, Y)$

Table 2 Ellipticity classes

F	θ	X	μ
$-\text{DtN}^+, \text{DtN}^-, \text{V}^{-1}, \text{W}$	$-\text{Arg}$	$H^{1/2}(\Gamma)$	1
$-\text{NtD}^+, \text{NtD}^-, \text{W}^{-1}, \text{V}$	Arg	$H^{-1/2}(\Gamma)$	2

The prototype is $F \in \mathcal{E}(\mu, \theta, X)$

4 The proof technique with a first example

In our analysis, to be able to transform discretized boundary integral equations (alone or coupled with FEM discretizations of interior problems) into non-standard transmission problems plays an important role. Let us introduce the notations that will allow us to do it in a systematic and hopefully optimal way.

Given an open set $\mathcal{O} \subset \mathbb{R}^d$ let us consider the operator $A_{\mathcal{O}}(s)$ defined from $H^1(\mathcal{O})$ into its dual by

$$\langle A_{\mathcal{O}}(s)u, v \rangle := \int_{\mathcal{O}} \nabla u \cdot \nabla v + s^2 \int_{\mathcal{O}} uv.$$

When $s = \delta > 0$ we have the norm

$$\|u\|_{\delta, \mathcal{O}} := \langle A_{\mathcal{O}}(\delta)u, \bar{u} \rangle^{1/2},$$

which is equivalent to the usual one. Note that $\| \cdot \|_{|s|, \mathcal{O}}$ can be interpreted as the total energy (potential plus kinetic) in the frequency domain.

Notation First of all, we will always write σ for the real part of s , so this substitution has to be done implicitly wherever σ appears. Also, we will write the truncated variable

$$a > 0 \quad \longmapsto \quad \underline{a} := \min\{1, a\}.$$

This truncation operator inherits these useful properties in monomial fashion

$$\underline{a}^k = (\underline{a})^k, \quad \underline{a}^{k+k'} = \underline{a}^k \underline{a}^{k'}, \quad k, k' > 0.$$

Because of the first property we will be able to write \underline{a}^k without ambiguity.

The energy norms can be easily related to the usual norms: for all $s \in \mathbb{C}_+$

$$\underline{\sigma} \|u\|_{1, \mathcal{O}} \leq \|u\|_{|s|, \mathcal{O}} \leq \frac{|s|}{\underline{\sigma}} \|u\|_{1, \mathcal{O}}, \quad \forall u \in H^1(\mathcal{O}), \tag{5}$$

where in the last inequality we have used that $\max\{1, |s|\} \min\{1, \sigma\} \leq |s|$ for all $s \in \mathbb{C}_+$. Also we have for all $s \in \mathbb{C}_+$:

$$|\langle A_{\mathcal{O}}(s)u, v \rangle| \leq \|u\|_{|s|, \mathcal{O}} \|v\|_{|s|, \mathcal{O}}, \quad \forall u, v \in H^1(\mathcal{O}). \tag{6}$$

Finally

$$\operatorname{Re} \left(e^{-i \operatorname{Arg} s} \langle A_{\mathcal{O}}(s)u, \bar{u} \rangle \right) = \frac{\sigma}{|s|} \|u\|_{|s|, \mathcal{O}}^2. \tag{7}$$

Lemma 5 *Let $\mathcal{O}_1, \dots, \mathcal{O}_p$ be open sets in \mathbb{R}^d and consider a closed subspace*

$$\widehat{H} \subset H^1(\mathcal{O}_1) \times \dots \times H^1(\mathcal{O}_p).$$

Let $\widehat{\gamma} : \widehat{H} \rightarrow \Xi$ be a surjective bounded linear map onto another Hilbert space Ξ , $\widehat{\gamma}^\dagger$ a linear bounded right-inverse of $\widehat{\gamma}$ and let \widehat{H}_0 be the kernel of $\widehat{\gamma}$. Finally, let

$$\langle A(s)u, v \rangle := \sum_{j=1}^p \langle A_{\mathcal{O}_j}(s)u_j, v_j \rangle, \quad u = (u_1, \dots, u_p), \quad v = (v_1, \dots, v_p).$$

Then for arbitrary $\ell \in \widehat{H}'$ and $\xi \in \Xi$, the unique solution of

$$\begin{cases} u \in \widehat{H}, & \widehat{\gamma}u = \xi, \\ \langle A(s)u, v \rangle = \langle \ell, v \rangle, & \forall v \in \widehat{H}_0, \end{cases} \tag{8}$$

satisfies the bound

$$\left(\sum_{j=1}^p \|u\|_{|s|, \mathcal{O}_j}^2 \right)^{1/2} \leq \frac{3|s|^2}{\sigma \underline{\sigma}^3} \left(\|\ell\| + 2\|\widehat{\gamma}^\dagger\| \|\xi\| \right) \tag{9}$$

The norms of ℓ , ξ and of the right-inverse $\widehat{\gamma}^\dagger$ are the ones of \widehat{H}' , Ξ and $\mathcal{L}(\Xi, \widehat{H})$, respectively.

Proof The existence and uniqueness of solution of (8) follow readily from (7) and the surjectivity of $\widehat{\gamma}$. The only estimate left to prove is thus (9). For notational simplicity we will use $\|\cdot\|_1$ for the product $H^1(\mathcal{O}_1) \times \dots \times H^1(\mathcal{O}_p)$ norm and $\|\cdot\|_{|s|}$ for the norm in the left-hand side of (9). Part of the argument is the usual one for elliptic boundary value problems with non-homogeneous essential conditions. First we solve the problem

$$\begin{cases} \widehat{u} \in \widehat{H}, & \widehat{\gamma}\widehat{u} = \xi, \\ \langle A(1)\widehat{u}, v \rangle = \langle \ell, v \rangle, & \forall v \in \widehat{H}_0. \end{cases}$$

This is accomplished by writing $\widehat{u} = \widehat{\gamma}^\dagger \xi + w_0$ with $w_0 \in \widehat{H}_0$ and using the ellipticity bound

$$\|w_0\|_1^2 = \langle A(1)w_0, \overline{w_0} \rangle = |\langle \ell, \overline{w_0} \rangle - \langle A(1)\widehat{\gamma}^\dagger \xi, \overline{w_0} \rangle| \leq \|w_0\|_1 \left(\|\ell\| + \|\widehat{\gamma}^\dagger\| \|\xi\| \right)$$

to obtain

$$\frac{\sigma}{|s|} \|\widehat{u}\|_{|s|} \leq \|\widehat{u}\|_1 \leq \|\ell\| + 2\|\widehat{\gamma}^\dagger\| \|\xi\|. \tag{10}$$

Second, we decompose $u = \widehat{u} + u_0$ where u_0 has to solve

$$\begin{cases} u_0 \in \widehat{H}_0, \\ \langle A(s)u_0, v \rangle = \langle (A(1) - A(s))\widehat{u}, v \rangle, \quad \forall v \in \widehat{H}_0. \end{cases}$$

Using (5)–(7) we obtain

$$\begin{aligned} \frac{\sigma}{|s|} \|u_0\|_{|s|}^2 &= \operatorname{Re} \left(e^{-i \operatorname{Arg} s} \langle A(s)u_0, \overline{u_0} \rangle \right) \leq |\langle (A(1) - A(s))\widehat{u}, \overline{u_0} \rangle| \\ &\leq \left(\frac{1}{\sigma^2} + 1 \right) \|\widehat{u}\|_{|s|} \|u_0\|_{|s|}. \end{aligned}$$

With this inequality, (5) and (10) we prove

$$\begin{aligned} \|u\|_{|s|} &\leq \|\widehat{u}\|_{|s|} + \|u_0\|_{|s|} \leq \left(1 + \frac{|s|}{\sigma} \left(\frac{1}{\sigma^2} + 1 \right) \right) \|\widehat{u}\|_{|s|} \\ &\leq \left(1 + \frac{|s|}{\sigma} \left(\frac{1}{\sigma^2} + 1 \right) \right) \frac{|s|}{\sigma} \left(\|\ell\| + 2\|\widehat{\gamma}^\dagger\| \|\xi\| \right). \end{aligned}$$

We can now simplify the constant in the previous inequality using the overestimates $\sigma \leq 1$ and $\sigma \leq |s|$ to obtain (9). □

We will use Lemma 5 with $p = 1$ or 2 , although some of the applications will admit different re-writings with more subdomains (we will often encounter the domain $\mathbb{R}^d \setminus \Gamma$, that can be split into Ω_- and Ω_+). The result can be easily extended to bilinear forms

$$\int_{\mathcal{O}} \kappa_0 \nabla u \cdot \nabla v + s^2 \int_{\mathcal{O}} \kappa_1 uv,$$

where $\kappa_0, \kappa_1, 1/\kappa_0, 1/\kappa_1 \in L^\infty(\mathcal{O})$ are positive. We only have to change the constants in (5), that depend on these coefficients and translate their influence to all other constants in the Lemma.

Our first example for showing the proof technique is to show the invertibility of the discrete version of an exterior symmetric Steklov–Poincaré (Dirichlet-to-Neumann) boundary integral operator. As we will use it, this method is too complicated for the exterior Dirichlet problem (both a direct and indirect method based on the invertibility of V are valid in this occasion), but we will use it to demonstrate how the method of proof works before dealing with the three situations of our interest.

Consider the scattering problem, given in the frequency domain

$$\begin{cases} \Delta u - s^2 u = 0, & \text{in } \Omega_+, \\ \gamma^+ u = -\gamma u_{\text{inc}}, \end{cases} \tag{11}$$

where u_{inc} is the Laplace transform of the trace of an incident wave that reaches the obstacle at time greater than zero. We want to emphasize once again that CQ is not a method of inversion of the Laplace transform and that data (the incident wave) is used in the time domain when discretized. If we denote $\phi := \gamma^+ u$ and $\lambda := \partial_\nu^+ u$, then the frequency domain version of Kirchhoff’s formula is Green’s Third Theorem for the solution of (11):

$$u = D(s)\phi - S(s)\lambda.$$

Therefore, by the jumps relations of potentials, we know that $(\lambda, \phi) \in H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)$ solves the equation

$$\mathbf{H}(s) \begin{bmatrix} \lambda \\ \phi \end{bmatrix} := \begin{bmatrix} V(s) & -(\frac{1}{2}I + K(s)) \\ (\frac{1}{2}I + K(s))^t & W(s) \end{bmatrix} \begin{bmatrix} \lambda \\ \phi \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} \tag{12}$$

with right-hand side $(d_1, d_2) = (\gamma u_{\text{inc}}, 0)$. Note first that for $s > 0$, the operator $\mathbf{H}(s)$ is elliptic but that this is not so obviously true anymore for non-real s , since $K^*(s) = K^t(\bar{s}) \neq K^t(s)$ and conjugations in the tests (therefore adjoints more that transposes) play a key role in the ellipticity estimates for $V(s)$ and $W(s)$ (see Appendix 2).

If $\mathbf{B}(s)$ is a $p \times p$ matrix of operators it is easy to prove that

$$\|\mathbf{B}(s)\| \leq p \max_{i,j} \|B_{ij}(s)\|. \tag{13}$$

Therefore, using the bounds for the integral operators, we obtain

$$\mathbf{H} \in \mathcal{A}(2, H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma), H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma)).$$

Proposition 6 For all $s \in \mathbb{C}_+$, $\mathbf{H}^{-1}(s)$ exists and

$$\mathbf{H}^{-1} \in \mathcal{A}\left(2, H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma), H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)\right).$$

Proof Using identities for the integral operators it is possible to prove that

$$\mathbf{H}^{-1}(s) = \begin{bmatrix} -DtN^+(s) & I \\ -I & NtD^-(s) \end{bmatrix}. \tag{14}$$

To see this in a direct way, we argue as follows. If (λ, ϕ) solves (12), then we can define $u := S(s)\lambda - D(s)\phi$ and we know that

$$\begin{cases} \Delta u - s^2 u = 0, & \text{in } \mathbb{R}^d \setminus \Gamma, \\ \gamma^+ u = d_1, \\ \partial_\nu^- u = d_2. \end{cases} \tag{15}$$

Now, (15) is just an interior Neumann problem together with an exterior Dirichlet problem. The jumps $[\partial_\nu u] = \lambda$ and $[\gamma u] = \phi$ can be recovered by solving these problems and it is then straightforward to see that

$$[\partial_\nu u] = d_2 - \partial_\nu^+ u = d_2 - DtN^+(s)d_1$$

and

$$[\gamma u] = \gamma^- u - d_1 = NtD^-(s)d_1 - d_2.$$

This proves (14). The needed bound can now be obtained using the results of Sect. 3 and (13). □

Let us now discretize Eq. (12). We take a sequence of finite-dimensional spaces

$$X_h \subset H^{-1/2}(\Gamma), \quad Y_h \subset H^{1/2}(\Gamma).$$

Given $g \in H^{1/2}(\Gamma)$, we denote $X_h^t g := \langle \cdot, g \rangle : X_h \rightarrow \mathbb{C}$. Similarly Y_h^t restricts the action of elements of $H^{-1/2}(\Gamma)$ to Y_h . Note that $X_h^t : H^{1/2}(\Gamma) \rightarrow X_h^t$ is the transpose of the natural inclusion of X_h into $H^{-1/2}(\Gamma)$. We now set the discrete equations of a Galerkin method

$$\begin{cases} (\lambda_h, \phi_h) \in X_h \times Y_h, \\ \langle \mu_h, \mathbf{V}(s)\lambda_h \rangle - \langle \mu_h, (\frac{1}{2}\mathbf{I} + \mathbf{K}(s))\lambda_h \rangle = \langle \mu_h, d_1 \rangle, \quad \forall \mu_h \in X_h, \\ \langle (\frac{1}{2}\mathbf{I} + \mathbf{K}(s))^t \lambda_h, \varphi_h \rangle + \langle \mathbf{W}(s)\phi_h, \varphi_h \rangle = \langle d_2, \varphi_h \rangle, \quad \forall \varphi_h \in Y_h, \end{cases}$$

that can be written in operator form as

$$\mathbf{H}_h(s) \begin{bmatrix} \lambda_h \\ \phi_h \end{bmatrix} := \begin{bmatrix} \mathbf{V}_h(s) & -(\frac{1}{2}\mathbf{I} + \mathbf{K}(s))_h \\ (\frac{1}{2}\mathbf{I} + \mathbf{K}(s))_h^t & \mathbf{W}_h(s) \end{bmatrix} \begin{bmatrix} \lambda_h \\ \phi_h \end{bmatrix} = \begin{bmatrix} X_h^t d_1 \\ Y_h^t d_2 \end{bmatrix}, \tag{16}$$

The remainder of this section is a proof of the following result.

Proposition 7 $\mathbf{H}_h^{-1} \in \mathcal{A}^{\text{unif}}(\frac{5}{2}, X_h' \times Y_h', X_h \times Y_h)$.

Proof We will do this proof in four steps.

Step 1 Take $(d_1, d_2) \in X_h' \times Y_h'$. If

$$\mathbf{H}_h(s)(\lambda_h, \phi_h)^\top = (d_1, d_2)^\top, \tag{17}$$

then the function $u = S(s)\lambda_h - D(s)\phi_h$ is a solution to the non-standard transmission/boundary value problem

$$\begin{cases} \Delta u - s^2u = 0, & \text{in } \mathbb{R}^d \setminus \Gamma, \\ [\gamma u] \in Y_h, \quad [\partial_\nu u] \in X_h, \\ X_h^t \gamma^+ u = d_1, \quad Y_h^t \partial_\nu^- u = d_2. \end{cases} \tag{18}$$

Reciprocally, if $u \in H^1(\mathbb{R}^d \setminus \Gamma)$ solves (18), then $([\partial_\nu u], [\gamma u])$ solves the discrete equations (17). Since solutions of $\Delta u - s^2u = 0$ in $\mathbb{R}^d \setminus \Gamma$ are characterized by the jumps of their Cauchy data on Γ (by Green’s Third Theorem), uniqueness of solution of each problem is implied by the other one.

Step 2 Consider the space $\widehat{H} := \{u \in H^1(\mathbb{R}^d \setminus \Gamma) \mid [\gamma u] \in Y_h\}$ and the operator $\widehat{\gamma} := X_h^t \gamma^+ : \widehat{H} \rightarrow X_h'$. Then

$$\widehat{H}_0 := \ker \widehat{\gamma} = \left\{ u \in H^1(\mathbb{R}^d \setminus \Gamma) \mid [\gamma u] \in Y_h, \quad \gamma^+ u \in X_h^\circ \right\},$$

X_h° being the polar set (or annihilator) of X_h . The *second step* consists of proving that (18) is equivalent to the following weak problem

$$\begin{cases} u \in \widehat{H}, \quad \widehat{\gamma} u = d_1, \\ \langle A_{\mathbb{R}^d \setminus \Gamma}(s)u, v \rangle = \langle d_2, [\gamma v] \rangle, \quad \forall v \in \widehat{H}_0. \end{cases} \tag{19}$$

If u solves this last problem, then using that $\mathcal{D}(\mathbb{R}^d \setminus \Gamma) \subset \widehat{H}_0$ it follows that $\Delta u - s^2u = 0$ in $\mathbb{R}^d \setminus \Gamma$ and using the definition of weak normal derivative (Green’s First Theorem),

$$\langle \partial_\nu^- u, \gamma^- v \rangle - \langle \partial_\nu^+ u, \gamma^+ v \rangle = \langle d_2, [\gamma v] \rangle, \quad \forall v \in \widehat{H}_0. \tag{20}$$

Let $\xi \in X_h^\circ$ and lift it to $v \in \widehat{H}^1(\mathbb{R}^d)$ such that $\gamma^\pm v = \xi$. Then (20) implies that

$$\langle [\partial_\nu u], \xi \rangle = 0, \quad \forall \xi \in X_h^\circ,$$

from where it follows that $[\partial_\nu u] \in X_h$. Finally, take $\varphi_h \in Y_h$ and construct $v \in H^1(\mathbb{R}^d \setminus \Gamma)$ in the following way: in Ω_+ we take $v \equiv 0$ and in Ω_- we take any lifting of φ_h . Inputting the resulting $v \in \widehat{H}_0$ in (20) we obtain

$$\langle \partial_\nu^- u, \varphi_h \rangle = \langle d_2, \varphi_h \rangle, \quad \forall \varphi_h \in Y_h,$$

i.e., $Y_h^t \partial_\nu^- u = d_2$. We have thus proved that u solves (18). For the reciprocal statement notice first that

$$\langle \partial_\nu^- u, \gamma^- v \rangle - \langle \partial_\nu^+ u, \gamma^+ v \rangle = \langle \partial_\nu^- u, [\gamma v] \rangle + \langle [\partial_\nu u], \gamma^+ v \rangle.$$

Then, if u is a solution to (18), it also satisfies (20). From this equation and the partial differential equation $\Delta u - s^2u = 0$, we easily arrive at the variational formulation (19).

Step 3 Given $\xi \in X_h'$ we can extend it to $\tilde{\xi} \in H^{1/2}(\Gamma) = (H^{-1/2}(\Gamma))'$ with $\|\tilde{\xi}\|_{1/2,\Gamma} = \|\xi\|$ by demanding

$$\tilde{\xi}|_{X_h} = \xi, \quad \tilde{\xi}|_{X_h^\perp} = 0, \tag{21}$$

X_h^\perp being the orthogonal complement to X_h . Now we take a continuous lifting $u := \gamma^{\dagger} \tilde{\xi} \in H^1(\mathbb{R}^d)$. Hence $\widehat{\gamma}$ is onto and we have a uniformly bounded right-inverse, so we are in the hypotheses of Lemma 5 and we have a unique solution to (18) and (19) satisfying

$$\|u\|_{|s|, \mathbb{R}^d \setminus \Gamma} \leq C(\sigma) |s|^2 (\|d_1\| + \|d_2\|). \tag{22}$$

We have therefore a solution to (17), which proves that $\mathbf{H}_h^{-1}(s)$ exists for all s .

Step 4 Using (63) in Appendix 2 as well as (5) we can bound

$$\begin{aligned} \|\lambda_h\|_{-1/2, \Gamma} + \|\phi_h\|_{1/2, \Gamma} &= \|[\partial_\nu u]\|_{-1/2, \Gamma} + \|[\gamma u]\|_{1/2, \Gamma} \\ &\leq C_\Gamma \left(\frac{|s|^{1/2}}{\underline{\sigma}^{1/2}} + \frac{1}{\underline{\sigma}} \right) \|u\|_{|s|, \mathbb{R}^d \setminus \Gamma}. \end{aligned}$$

From this and (22) we obtain the necessary bound to prove the statement of the Proposition. □

There is an interesting and somewhat unexpected by-product of this form of analysis. Usually one concentrates in the discretization of the boundary integral system, but we also have to take into account the postprocessing of the solution to obtain the exterior solution. In the context of CQ methods, this means that we apply the method for the boundary integral equations and then plug the result into the retarded potential expression, which is again discretized using CQ. In the frequency domain this is just

$$\begin{bmatrix} -S(s) & D(s) \end{bmatrix} \mathbf{H}_h^{-1}(s) \begin{bmatrix} X_h^I u_{\text{inc}} \\ 0 \end{bmatrix}.$$

Because CQ is a discrete operational calculus, if we have a bound in s for the operator in the previous expression, we obtain the behavior for the progressive application of the solution of the boundary integral system and the potential postprocessing. If we apply the composition rule (1) and Proposition 7, we end up with an index $\mu = \frac{5}{2} + 2$. However, the operator $\begin{bmatrix} S(s) & -D(s) \end{bmatrix} \mathbf{H}_h^{-1}(s)$ gives precisely u in the proof of Proposition 7 and therefore, using (9) and (5) we have proved that

$$\begin{bmatrix} -S & D \end{bmatrix} \mathbf{H}_h^{-1} \in \mathcal{A}^{\text{unif}} \left(2, X'_h \times Y'_h, H^1(\Omega_+) \right).$$

5 Mixed exterior boundary conditions

Consider now the following exterior mixed scattering problem, written again in the frequency domain:

$$\begin{cases} \Delta u - s^2 u = 0, & \text{in } \Omega_+, \\ \gamma^+ u = -\gamma u_{\text{inc}}, & \text{on } \Gamma_D, \\ \partial_\nu^+ u = -\partial_\nu u_{\text{inc}}, & \text{on } \Gamma_N. \end{cases} \tag{23}$$

The sets Γ_D, Γ_N form a non-overlapping conforming partition of the boundary Γ with the usual Lipschitz requirements. This problem arises when the scatterer is composed of several disjoint obstacles some of which are sound-soft (Dirichlet conditions), the others being sound-hard (Neumann conditions). We will accept anyway the case in which the boundary of a scatterer is part Dirichlet, part Neumann since it does not influence our analysis.

We will proceed following an idea that is a slight modification of the coupling method in [39]. First of all we assume that we have extended the Dirichlet and Neumann data to the whole boundary, so we are given $g_1 \in H^{1/2}(\Gamma)$ and $g_2 \in H^{-1/2}(\Gamma)$ that extend the boundary values we want to impose. If the Dirichlet/Neumann decomposition corresponds to boundaries of different scatterers we can extend the data by zero. Given the fact that data are traces from an incident wave it is even simpler to use the full traces of the incident wave as extended boundary values.

The unknowns will be

$$\phi := \gamma^+ u - g_1 \in Y_N := \left\{ \phi \in H^{1/2}(\Gamma) \mid \phi \equiv 0, \text{ in } \Gamma_D \right\} \tag{24}$$

and

$$\begin{aligned} \lambda := \partial_\nu^+ u - g_2 \in X_D := & \left\{ \lambda \in H^{-1/2}(\Gamma) \mid \lambda = 0, \text{ in } \Gamma_N \right\} \\ & = \left\{ \lambda \in H^{-1/2}(\Gamma) \mid \langle \lambda, \varphi \rangle = 0, \forall \varphi \in Y_N \right\}. \end{aligned} \tag{25}$$

Note that Y_N is isomorphic to $H_0^{1/2}(\Gamma_N)$ (elements of $H^{1/2}(\Gamma_N)$ that can be extended by zero) and X_D is isomorphic to the dual space of $H^{1/2}(\Gamma_D)$. We can then use the symmetric identities

$$\begin{aligned} \mathbb{V}(s) \partial_\nu^+ u - \left(\frac{1}{2} \mathbb{I} + \mathbb{K}(s) \right) \gamma^+ u &= -\gamma^+ u, \\ \left(\frac{1}{2} \mathbb{I} + \mathbb{K}(s) \right)^t \partial_\nu^+ u + \mathbb{W}(s) \gamma^+ u &= 0 \end{aligned}$$

substitute $\gamma^+ u = \phi + g_1, \partial_\nu^+ u = \lambda + g_2$, test the first equation with X_D and the second one with Y_N . Using the definition of X_D and Y_N , we see that $X_D^t \phi = 0$ and therefore the term that appears in right-hand side of the first equation is simply $-X_D^t g_1 = \gamma u_{\text{inc}}$. Note that time operators affect the data and we have to take that into account in the full analysis. We will even consider the possibility of discretizing data in space.

We will cover at the same time several situations, continuous and discrete in a unified analysis. We need four closed spaces: two for unknowns (subscripted with u) and two for data (subscripted with d)

$$X_u, X_d \subset H^{-1/2}(\Gamma), \quad Y_u, Y_d \subset H^{1/2}(\Gamma).$$

Writing $X_\alpha : X_\alpha \rightarrow H^{-1/2}(\Gamma)$ and $Y_\alpha : Y_\alpha \rightarrow H^{1/2}(\Gamma)$ for the inclusion operators with $\alpha \in \{u, d\}$, we can define the operators

$$\mathbf{H}_{u\alpha}(s) := \begin{bmatrix} X_u^t & 0 \\ 0 & Y_u^t \end{bmatrix} \mathbf{H}(s) \begin{bmatrix} X_\alpha & 0 \\ 0 & Y_\alpha \end{bmatrix} : X_\alpha \times Y_\alpha \rightarrow X'_u \times Y'_u, \quad \alpha \in \{u, d\},$$

where $\mathbf{H}(s)$ is the operator of (12). The general equations are

$$\begin{bmatrix} \mathbf{H}_{uu}(s) & \mathbf{H}_{ud}(s) \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \lambda_u \\ \phi_u \\ \lambda_d \\ \phi_d \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \end{bmatrix}. \tag{26}$$

Before going any further, let us detail several different examples that fit into this frame.

- (a) We take $Y_u = Y_N$ and $X_u = X_D$, the spaces of (24) and (25), plus $X_d = H^{1/2}(\Gamma)$ and $Y_d = H^{-1/2}(\Gamma)$. Equations (26) with right-hand side $(-X_u^t g_1, 0, g_2, g_1)$ are the ones of the mixed problem. Recall that $-X_D^t g_1$ is equal to the value of γu_{inc} on Γ_D .
- (b) If $X_u = X_h \subset X_D$ and $Y_u = Y_h \subset Y_N$ are finite-dimensional, we leave the other two spaces as in (a) and take the same right-hand side, we are dealing with a discretization of the equations for the mixed exterior boundary value problem.
- (c) With the same choice for the spaces X_u and Y_u as in (b) and taking finite-dimensional spaces $X_d^h \subset H^{-1/2}(\Gamma)$ and $Y_d^h \subset H^{1/2}(\Gamma)$, we are dealing with a discrete model that projects the incoming data into discrete subspaces before inputting them into the potentials. In the mixed problem that motivates this section, the right-hand side is constructed as follows. We need two uniformly bounded projections

$$P_h : H^{-1/2}(\Gamma) \rightarrow X_d^h, \quad Q_h : H^{1/2}(\Gamma) \rightarrow Y_d^h. \tag{27}$$

The right-hand side is then $(-X_u^t Q_h g_1, 0, P_h g_2, Q_h g_1)$. This kind of projection of data into discrete spaces is the Galerkin version of what is usually done in the engineering literature of BEM: treating data as unknowns and then substituting their known values at the final step [34].

- (d) We can take $X_u = H^{-1/2}(\Gamma)$, $Y_u = \{0\}$, $X_d = \{0\}$ and $Y_d = H^{1/2}(\Gamma)$. In this case we are analyzing an integral formulation for the exterior Dirichlet problem using the first integral identity

$$V(s)\lambda_u + (\frac{1}{2}\mathbf{I} - \mathbf{K}(s))\phi_d = 0, \quad \phi_d = g.$$

The non-trivial spaces can be discretized (only X_u or both of them) corresponding to Galerkin discretization of the equation with or without discretization of data.

(e) We can deal with the opposite situation by taking $X_u = \{0\}$, $Y_u = H^{1/2}(\Gamma)$, $X_d = H^{-1/2}(\Gamma)$, $Y_d = \{0\}$. In this case, we are using the second integral identity

$$W(s)\phi_u + (\frac{1}{2}I + K(s))^t \lambda_d = 0, \quad \lambda_d = g,$$

for the exterior Neumann problem. Discretization of this case can also be accomplished as in (d), be it only for the unknown ϕ_u or for the copy of the data too.

Other choices of the four spaces (that are completely free) lead to more or less exotic transmission/BVP problems in $\mathbb{R}^d \setminus \Gamma$.

Let us denote by $\mathbf{H}_{\text{mix}}(s)$ the operator in (26). By (13) and the bounds collected in Sect. 3, it follows that

$$\mathbf{H}_{\text{mix}} \in \mathcal{A}(2, X_u \times Y_u \times X_d \times Y_d, X'_u \times Y'_u \times X_d \times Y_d)$$

and the constants can be taken independent of the choice of the four spaces.

Proposition 8 *The operator $\mathbf{H}_{\text{mix}}(s)$ is invertible for all $s \in \mathbb{C}_+$ and*

$$\mathbf{H}_{\text{mix}}^{-1} \in \mathcal{A}\left(\frac{5}{2}, X'_u \times Y'_u \times X_d \times Y_d, X_u \times Y_u \times X_d \times Y_d\right).$$

All constants in the bounds can be taken independent of the choice of the spaces, so in the discrete case we have elements of the uniform classes. Finally the operator

$$\begin{bmatrix} S(s) & -D(s) \end{bmatrix} \begin{bmatrix} X_u & 0 & X_d & 0 \\ 0 & Y_u & 0 & Y_d \end{bmatrix} \mathbf{H}_{\text{mix}}^{-1}(s) \tag{28}$$

belongs to $\mathcal{A}(2, X'_u \times Y'_u \times X_d \times Y_d, H^1(\Omega_+))$ with constants independent of the choice of the spaces.

Proof Let $(\lambda_u, \phi_u, \lambda_d, \phi_d)$ solve (26). Then

$$u := S(s)(\lambda_u + \lambda_d) - D(s)(\phi_u + \phi_d) \tag{29}$$

satisfies

$$\begin{cases} \Delta u - s^2 u = 0, & \text{in } \mathbb{R}^d \setminus \Gamma, \\ X_u^t \gamma^+ u = d_1, & Y_u^t \partial_\nu^- u = d_2, \\ [\partial_\nu u] - d_3 \in X_u, & [\gamma u] - d_4 \in Y_u. \end{cases} \tag{30}$$

Reciprocally, given a solution u of (30), the function

$$([\partial_\nu u] - d_3, [\gamma u] - d_4, d_3, d_4)$$

solves (26). The fourth condition of (30) (second of the transmission conditions) has to be written in weak form to fit our general frame. To do that we simply remark that this condition is equivalent to

$$(Y_u^\circ)^t[\gamma u] = (Y_u^\circ)^t d_4,$$

where $Y_u^\circ : Y_u^\circ \rightarrow H^{-1/2}(\Gamma)$ is, as usual, the canonical inclusion. With these elements in hand, we take now $\widehat{H} := H^1(\mathbb{R}^d \setminus \Gamma)$, $\widehat{\gamma} : \widehat{H} \rightarrow X'_u \times (Y_u^\circ)'$ given by

$$\widehat{\gamma}u := (X'_u \gamma^+ u, (Y_u^\circ)^t[\gamma u]),$$

so that

$$\widehat{H}_0 = \left\{ v \in H^1(\mathbb{R}^d \setminus \Gamma) \mid \gamma^+ v \in X_u^\circ, \quad [\gamma v] \in Y_u \right\}.$$

Then (30) is shown to be equivalent to

$$\begin{cases} u \in \widehat{H}, & \widehat{\gamma}u = (d_1, (Y_u^\circ)^t d_4), \\ \langle A_{\mathbb{R}^d \setminus \Gamma}(s)u, v \rangle = \langle d_3, \gamma^+ v \rangle + \langle d_2, [\gamma v] \rangle, & \forall v \in \widehat{H}_0. \end{cases} \tag{31}$$

Before going any further, let us remark that the choice of X_u and Y_u is immaterial in all the preceding arguments. A right-inverse for $\widehat{\gamma}$, with bound independent of what the spaces are, is easy to obtain. If we want to find $u \in \widehat{H}$ such that $\widehat{\gamma}u = (\xi, \eta) \in X'_u \times (Y_u^\circ)'$, following the construction in (21), we first extend ξ and η to $\widetilde{\xi}, \widetilde{\eta} \in H^{1/2}(\Gamma)$ preserving the respective norms. We then proceed to take $u \in H^1(\Omega_+)$ such that $\gamma^+ u = \widetilde{\xi}$ and $u \in H^1(\Omega_-)$ such that $\gamma^- u = \widetilde{\xi} + \widetilde{\eta}$, using a continuous lifting operator on each side of Γ . This provides a linear bounded right-inverse of $\widehat{\gamma}$.

The remainder of the proof consists of using Lemma 5 and then bounding the jump of the trace and of the normal derivative of u that are needed to reconstruct λ_u and ϕ_u . Finally the bound for the operator (28) is obtained as in Sect. 4, since the effect of applying this operator is precisely the result of solving the Eq. (26) and then constructing u with (29). □

6 Non-homogeneous penetrable obstacles (1)

Consider now a transmission problem, written in the frequency domain:

$$\begin{cases} \nabla \cdot (\kappa_0 \nabla u) - s^2 \kappa_1 u = 0, & \text{in } \Omega_-, \\ [\gamma u] = \gamma u_{\text{inc}}, \\ \kappa_0 \partial_\nu^- u - \partial_\nu^+ u = \partial_\nu u_{\text{inc}}, \\ \Delta u - s^2 u = 0, & \text{in } \Omega_+. \end{cases} \tag{32}$$

Here $\kappa_0, \kappa_1 \in L^\infty(\Omega_-)$ are strictly positive functions, so that $1/\kappa_0, 1/\kappa_1 \in L^\infty(\Omega_-)$. The interior flux $\kappa_0 \partial_\nu^- u$ is defined similarly to the normal derivative. We can now use the representation for the exterior solution (60), write

$$\lambda := \partial_\nu^+ u, \quad \phi := \gamma^+ u \tag{33}$$

and leave the name u for the part of the unknown defined in the interior domain. With some abuse of notation (see the comments after the proof of Lemma 5), we will not change the name for the operator in the interior domain

$$\langle A_{\Omega_-}(s)u, v \rangle := \int_{\Omega_-} \kappa_0 \nabla u \cdot \nabla v + s^2 \int_{\Omega_-} \kappa_1 u v.$$

We will use the symbol γ for the traces of functions defined only in Ω_- , where there is no doubt of whether there is an interior or exterior trace since there is no exterior component. Using the identities for the Cauchy data of the exterior solution (60) we see that (u, λ, ϕ) solves

$$\begin{bmatrix} A_{\Omega_-}(s) & -\gamma^t & 0 \\ \gamma & V(s) & -(\frac{1}{2}I + K(s)) \\ 0 & (\frac{1}{2}I + K(s))^t & W(s) \end{bmatrix} \begin{bmatrix} u \\ \lambda \\ \phi \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix} \tag{34}$$

with $(d_1, d_2, d_3) = (\gamma^t \partial_\nu u_{inc}, \gamma u_{inc}, 0)$. This coupling procedure yields a symmetric operator system (change the sign of the second row to obtain symmetry and recall (4)). It is a variant of the symmetric coupling of [8, 19] that can be found in [6] in the context of coupling non-conforming FEM and BEM.

A small digression. Before performing the corresponding discrete analysis (which will include a bound for the continuous operator as in the preceding section), let us display a decomposition of the boundary-field operator of (34), henceforth denoted $\mathbf{H}_{bf}(s)$. Gaussian elimination and scaling of the rows and columns of the operator produce a simpler form of $\mathbf{H}_{bf}(s)$, where the hidden ellipticity is recovered. Indeed, taking

$$\mathbf{P}(s) := \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & \text{NtD}^+(s) & I \end{bmatrix},$$

and using two of the identities for NtD^+ given in (58) we have the decomposition

$$\mathbf{P}(s)^t \begin{bmatrix} A_{\Omega_-}(s) & -\gamma^t & 0 \\ \gamma & -\text{NtD}^+(s) & 0 \\ 0 & 0 & W(s) \end{bmatrix} \mathbf{P}(s) = \mathbf{H}_{bf}(s).$$

If we consider a diagonal scaling matrix $\mathbf{D}(s) = \text{diag}(e^{t(\text{Arg}s)/2}I, e^{-t(\text{Arg}s)/2}I, e^{t(\text{Arg}s)/2}I)$, we can proceed further in the decomposition to obtain $\mathbf{H}_{bf}(s) = \mathbf{P}^t(s)\mathbf{D}^t(s)\mathbf{C}(s)\mathbf{D}(s)\mathbf{P}(s)$ with

$$C(s) := \begin{bmatrix} e^{-t \operatorname{Arg} s} A_{\Omega_-}(s) & -\gamma^t & 0 \\ \gamma & e^{t \operatorname{Arg} s} \operatorname{NtD}^-(s) & 0 \\ 0 & 0 & e^{-t \operatorname{Arg} s} W(s) \end{bmatrix}.$$

Using (7), Propositions 17 and 19 we can prove that

$$\operatorname{Re} \langle C(s)(u, \lambda, \phi), (\bar{u}, \bar{\lambda}, \bar{\phi}) \rangle \geq C(\operatorname{Re} s) |s|^{-2} \|(u, \lambda, \phi)\|^2,$$

which can be used to give a bound for the inverse of \mathbf{H}_{bf} . Note however, that when inverting the operators \mathbf{P} and \mathbf{P}^t the parameter μ is increased by the composition rule (1). This fact produces a clear overestimate of the ‘order’ of the inverse that we will be able to avoid using our strategy for analysis.

Take now three arbitrary families of finite-dimensional subspaces

$$V_h \subset H^1(\Omega_-), \quad X_h \subset H^{-1/2}(\Gamma), \quad Y_h \subset H^{1/2}(\Gamma)$$

and consider the discrete equations

$$\begin{bmatrix} A_{\Omega_-}^h(s) & -\gamma_h^t & 0 \\ \gamma_h & V_h(s) & -(\frac{1}{2}I + K(s))_h \\ 0 & (\frac{1}{2}I + K(s))_h^t & W_h(s) \end{bmatrix} \begin{bmatrix} u_h \\ \lambda_h \\ \phi_h \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix} \tag{35}$$

for a general right-hand side in $V'_h \times X'_h \times Y'_h$. Let us denote by $\mathbf{H}_{\text{bf},h}(s)$ the operator in (35). For the sake of clarity and for the last time in this article, let us write the discrete equations corresponding to (35) when the right-hand side is the discrete version of $(\gamma^t \partial_\nu u_{\text{inc}}, \gamma u_{\text{inc}}, 0)$:

$$\left[\begin{array}{l} (u_h, \lambda_h, \phi_h) \in V_h \times X_h \times Y_h, \\ \langle A_{\Omega_-}(s)u_h, v_h \rangle - \langle \lambda_h, \gamma v_h \rangle = \langle \partial_\nu u_{\text{inc}}, \gamma v_h \rangle, \\ \langle \mu_h, \gamma u_h \rangle + \langle \mu_h, V(s)\lambda_h \rangle - \langle \mu_h, (\frac{1}{2}I + K(s))\phi_h \rangle = \langle \mu_h, \gamma u_{\text{inc}} \rangle, \\ \langle \lambda_h, (\frac{1}{2}I + K(s))\phi_h \rangle + \langle W(s)\phi_h, \phi_h \rangle = 0, \\ \forall (v_h, \mu_h, \phi_h) \in V_h \times X_h \times Y_h. \end{array} \right.$$

As usual this is a space discretization in the frequency domain, corresponding to a space discretization of a time-dependent equation that involves retarded integral equations and the second time derivative in the interior (FEM) domain. The unknown in the exterior domain is recovered with the formula $D(s)\phi_h - S(s)\lambda_h$ that involves the retarded potentials.

Proposition 9 *For any choice of the subspaces, $\mathbf{H}_{\text{bf},h}(s)$ is invertible for all $s \in \mathbb{C}_+$. Moreover,*

$$\mathbf{H}_{\text{bf},h}^{-1} \in \mathcal{A}^{\text{unif}} \left(\frac{5}{2}, V'_h \times X'_h \times Y'_h, V_h \times X_h \times Y_h \right)$$

and

$$\mathbf{H}_{\text{bf}}^{-1} \in \mathcal{A} \left(\frac{5}{2}, H^1(\Omega_-)' \times H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma), H^1(\Omega_-) \times H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma) \right)$$

Finally the operator that associates to given right-hand sides the interior and exterior fields

$$\begin{bmatrix} \mathbf{I} & 0 & 0 \\ 0 & -\mathbf{S}(s) & \mathbf{D}(s) \end{bmatrix} \mathbf{H}_{\text{bf},h}^{-1}(s) \tag{36}$$

belongs to $\mathcal{A}^{\text{unif}}(2, V_h' \times X_h' \times Y_h', V_h \times H^1(\Omega_+))$.

Proof We follow the four step program. *First* of all, given a solution to (35) we define

$$u^* := \mathbf{S}(s)\lambda_h - \mathbf{D}(s)\phi_h$$

and notice that the pair $(u_h, u^*) \in V_h \times H^1(\mathbb{R}^d \setminus \Gamma)$ solves the problem

$$\begin{cases} \Delta u^* - s^2 u^* = 0, & \text{in } \mathbb{R}^d \setminus \Gamma, \\ [\partial_\nu u^*] \in X_h, & [\gamma u^*] \in Y_h, \\ X_h^t(\gamma u_h + \gamma^+ u^*) = d_2, & Y_h^t \partial_\nu^- u^* = d_3, \\ A_{\Omega_-}^h(s)u_h - \gamma_h^t[\partial_\nu u^*] = d_1, \end{cases} \tag{37}$$

where the operators X_h^t and Y_h^t are defined as usual. Reciprocally, given a solution (u_h, u^*) of (37) the triplet $(u_h, [\partial_\nu u^*], [\gamma u^*])$ solves (35). *Second*, we define the closed space where we will look for the pair $u := (u_h, u^*)$

$$\widehat{H} := V_h \times \left\{ u^* \in H^1(\mathbb{R}^d \setminus \Gamma) \mid [\gamma u^*] \in Y_h \right\},$$

the abstract trace

$$\widehat{\gamma}u = \widehat{\gamma}(u_h, u^*) := X_h^t(\gamma u_h + \gamma^+ u^*) \in X_h'$$

(which is just taking $\gamma u_h + \gamma^+ u^*$ and testing it with elements of X_h) and its kernel \widehat{H}_0 . We then show that (37) is equivalent to

$$\begin{cases} u = (u_h, u^*) \in \widehat{H}, & \widehat{\gamma}u = d_2, \\ \langle A(s)u, v \rangle = \langle d_1, v_h \rangle + \langle d_3, [\gamma v^*] \rangle, & \forall v = (v_h, v^*) \in \widehat{H}_0, \end{cases} \tag{38}$$

where in the context of the abstract lemma of Sect. 2, $\mathcal{O}_1 := \Omega_-$ and $\mathcal{O}_2 := \mathbb{R}^d \setminus \Gamma$. Since this is somewhat more involved than what we have done in Sects. 4 and 5, we are going to detail one of the implications. Given a solution of (38), we can test it with $(0, v^*) \in \{0\} \times \mathcal{D}(\mathbb{R}^d \setminus \Gamma) \subset \widehat{H}_0$ to obtain the first equation of (37). Applying Green's First Theorem we obtain that

$$\langle A_{\Omega_-}(s)u_h, v_h \rangle + \langle \partial_\nu^- u^*, [\gamma v^*] \rangle + \langle [\partial_\nu u^*], \gamma^+ v^* \rangle = \langle d_1, v_h \rangle + \langle d_3, [\gamma v^*] \rangle, \tag{39}$$

for all $(v_h, v^*) \in \widehat{H}_0$. We now take $v_h = 0$ and $\gamma^+ v^* = \gamma^- v^*$ equalling an arbitrary element $\xi \in X_h^\circ$ to prove, from (39), that

$$\langle [\partial_\nu u^*], \xi \rangle = 0, \quad \forall \xi \in X_h^\circ,$$

and therefore $[\partial_\nu u^*] \in X_h$. Using this together with the fact that $\gamma v_h + \gamma^+ v^* \in X_h^\circ$, we further transform (39) into

$$\langle A_{\Omega_-}(s)u_h, v_h \rangle + \langle \partial_\nu^- u^*, [\gamma v^*] \rangle - \langle [\partial_\nu u^*], \gamma v_h \rangle = \langle d_1, v_h \rangle + \langle d_3, [\gamma v^*] \rangle, \quad (40)$$

for all $(v_h, v^*) \in \widehat{H}_0$. We are now free to take again $v_h = 0$ and v^* such that $[\gamma v^*]$ is any element of Y_h , to prove that $Y_h^t \partial_\nu^- u^* = d_3$, which allows to simplify (40) and prove the remaining equation in (37).

Third, we apply Lemma 5 to problem (38). To do that we need to create a right-inverse of $\widehat{\gamma}$. This can be done as in the proof of Proposition 8 (the interior discrete component u_h can be set to zero) with a bound independent of h . Then

$$\|u_h\|_{|s|, \Omega_-} + \|u^*\|_{|s|, \mathbb{R}^d \setminus \Gamma} \leq C(\sigma)|s|^2 \|(d_1, d_2, d_3)\|.$$

Using (5), this gives a proof of the bound for the operator in (36). *Fourth* and final, a simple application of (63) gives a bound for the reconstructed variables λ_h and ϕ_h and proves the result for the discrete operator.

Because the finite-dimensionality of the spaces is never used (only the fact that they are closed is important), the proof still holds when we take $V_h = H^1(\Omega_-)$, $X_h = H^{-1/2}(\Gamma)$ and $Y_h = H^{1/2}(\Gamma)$. We thus obtain the bound for the continuous operator. □

Note that unlike in the expression (28), we have omitted the inclusion operators in (36), since in this case the expressions are more self-explanatory. (Note also that in Sect. 5, even the continuous spaces were subspaces of the spaces $H^{\pm 1/2}(\Gamma)$). We will keep this simplified notation for all the forthcoming sections.

7 Non-homogeneous penetrable obstacles (2)

We go back to the transmission problem (32) and show two alternative ways of formulating the coupling, both having in common the non-duplication of the trace on the transmission interface (in the previous section ϕ_h and γu_h are essentially approximating the same quantity, up to the jump given by the incident wave). This amounts to going back to the coupling procedure of [8] or [19]. There is going to be a crucial difference with [8, 19], which will provoke the duality of approaches. The original coupling procedures were constructed for problems with homogeneous transmission conditions and did not have to take into account the fact that data are affected by integral operators. Since all operators that depend on s have to be discretized in time, we will have to deal with this effect. An alternative formulation to (34) at the continuous level consists of solving

$$\begin{bmatrix} A_{\Omega_-}(s) & -\gamma^t(\frac{1}{2}I - K(s))^t & \gamma^t W(s) \\ 0 & V(s) & \frac{1}{2}I - K(s) \\ \gamma & 0 & -I \end{bmatrix} \begin{bmatrix} u \\ \lambda \\ \phi \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix}. \tag{41}$$

with $(d_1, d_2, d_3) = (\gamma^t \partial_\nu u_{inc}, 0, \gamma u_{inc})$ and the unknowns as in Sect. 6. One of these, namely ϕ , can be easily eliminated from the coupled system and we obtain (in the particular case of the right-hand side of the scattering problem)

$$\begin{bmatrix} A(s) + \gamma^t W(s)\gamma & -\gamma^t(\frac{1}{2}I - K(s))^t \\ (\frac{1}{2}I - K(s))\gamma & V(s) \end{bmatrix} \begin{bmatrix} u \\ \lambda \end{bmatrix} = \begin{bmatrix} \gamma^t \partial_\nu u_{inc} + \gamma^t W(s)\gamma u_{inc} \\ (\frac{1}{2}I - K(s))\gamma u_{inc} \end{bmatrix}. \tag{42}$$

Note that γu_{inc} is affected by two integral operators that will have to be approximated in the time domain. Therefore, we proceed as in Sect. 5 and add an unknown ϕ_d that will deal with data under the action of integral operators. We are then led to studying systems of the form

$$\begin{bmatrix} A(s) + \gamma^t W(s)\gamma & -\gamma^t(\frac{1}{2}I - K(s))^t & -\gamma^t W(s) \\ (\frac{1}{2}I - K(s))\gamma & V(s) & -(\frac{1}{2}I - K(s)) \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} u \\ \lambda \\ \phi_d \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix}, \tag{43}$$

with $(d_1, d_2, d_3) = (\gamma^t \partial_\nu u_{inc}, 0, \gamma u_{inc})$. All the dependence on s is in the operator again. We will study both (41) and (43) and the continuous and discrete levels.

Let us begin with (41). For discretization we will use the spaces

$$V_h \subset H^1(\Omega_-), \quad X_h \subset H^{-1/2}(\Gamma), \quad Y_h := \gamma V_h \subset H^{1/2}(\Gamma).$$

Note that the space for the last unknown is just the trace space of the interior (Finite Element) space V_h . The discrete equations are:

$$\begin{bmatrix} A_{\Omega_-}^h(s) & -\gamma_h^t(\frac{1}{2}I - K(s))_h^t & \gamma_h^t W_h(s) \\ 0 & V_h(s) & (\frac{1}{2}I - K(s))_h \\ \gamma & 0 & -I \end{bmatrix} \begin{bmatrix} u_h \\ \lambda_h \\ \phi_h \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix}. \tag{44}$$

In the case of the scattering problem, the discrete right-hand side is $(\gamma_h^t \partial_\nu^+ u_{inc}, 0, Q_h \gamma^+ u_{inc})$, where $Q_h : H^{1/2}(\Gamma) \rightarrow Y_h$ is a stable projection onto Y_h (i.e., a projection with norm bounded independently of h). Note that from the point of view of implementation we can easily obtain a simpler scheme with only two unknowns, resembling (42), since the variable ϕ_h can be eliminated from the system. The last equation in (44) as well as the last one in (41) are not discretized or tested by any space, but taken at face value. Actually, it is the right-hand side that has to be preprocessed.

Proposition 10 *Let $\mathbf{H}_{\text{bf}2,h}(s)$ be the operator of Eq. (44). Then*

$$\mathbf{H}_{\text{bf}2,h}^{-1} \in \mathcal{A}^{\text{unif}} \left(\frac{5}{2}, V'_h \times X'_h \times Y_h, V_h \times X_h \times Y_h \right).$$

If $\mathbf{H}_{\text{bf}2}(s)$ is the operator of Eq. (41), then

$$\mathbf{H}_{\text{bf}2}^{-1} \in \mathcal{A} \left(\frac{5}{2}, H^1(\Omega_-)' \times H^{1/2}(\Gamma) \times H^{1/2}(\Gamma), H^1(\Omega_-) \times H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma) \right).$$

Finally the operator constructed by using the expression (36) with $\mathbf{H}_{\text{bf}2,h}(s)$ in place of $\mathbf{H}_{\text{bf},h}(s)$ has the same property as the one in Proposition 9.

Proof We will simply point out the milestones in the process of proof. Details can be filled by following carefully the proof of Proposition 9. Given a solution of (44) for $(d_1, d_2, d_3) \in V'_h \times X'_h \times Y_h$, we define $u^* = \mathbf{S}(s)\lambda_h - \mathbf{D}(s)\phi_h$ and prove that the pair (u_h, u^*) satisfies the transmission problem

$$\begin{cases} \Delta u^* - s^2 u^* = 0, & \text{in } \mathbb{R}^d \setminus \Gamma, \\ [\partial_\nu u^*] \in X_h, & [\gamma u^*] \in Y_h, \\ \gamma u_h - [\gamma u^*] = d_3, & X_h^t \gamma^- u^* = d_2, \\ A_{\Omega_-}^h(s)u_h + \gamma_h^t \partial_\nu^+ u^* = d_1. \end{cases} \tag{45}$$

Reciprocally, a solution to (45) gives another one for (44) by taking $\lambda_h := [\partial_\nu u^*]$ and $\phi_h := [\gamma u^*]$. The space for the weak formulation of (45) is

$$\widehat{H} := V_h \times \left\{ u^* \in H^1(\mathbb{R}^d \setminus \Gamma) \mid [\gamma u^*] \in Y_h \right\}.$$

The essential conditions are given by the trace operator

$$\widehat{\gamma}(u_h, u^*) := (X_h^t \gamma^- u^*, \gamma u_h - [\gamma u^*]) \in X'_h \times Y_h,$$

which admits a uniformly bounded right-inverse. The weak formulation is then

$$\begin{cases} u \in \widehat{H}, & \widehat{\gamma}u = (d_2, d_3), \\ \langle A(s)u, v \rangle = \langle d_3, v_h \rangle, & \forall v = (v_h, v^*) \in \widehat{H}_0. \end{cases}$$

What is left to be done about the discrete operator goes on as usual. Because the finite-dimensionality of the spaces does not play any role in the preceding argument, everything works with $V_h = H^1(\Omega_-)$, $X_h = H^{-1/2}(\Gamma)$ and $Y_h = H^{1/2}(\Gamma)$ and we obtain the bound for the continuous operator. \square

We now move to the Galerkin discretization of (43). We take two sequences of spaces $V_h \subset H^1(\Omega_-)$ and $X_h \subset H^{-1/2}(\Gamma)$ and a third space $Y_d \subset H^{1/2}(\Gamma)$. There are several options for this last space. If we do not want to discretize in space the incoming data, we take Y_d to be the full $H^{1/2}(\Gamma)$. A second option consists of taking $Y_d = \gamma V_h$. It is possible to prove that the resulting system is equivalent to (44). The

relationship between the variables is simply $\phi_d = \gamma u_h - \phi_h$. Finally Y_d can be an element of a sequence of discrete spaces completely independent of the other pair and in that case, the third component of the exact data for the scattering problem $d_3 = \gamma u_{inc}$ has to be projected onto Y_d in a stable way.

Proposition 10 holds for this new discrete operator that, as already mentioned, generalizes the previous choice. We are not going to develop all the details and simply show the main steps. The auxiliary function is

$$u^* = S(s)\lambda_h - D(s)(\gamma u_h + \phi_d).$$

Therefore, the variables on the boundary (λ_h, ϕ_d) can be easily recovered from knowledge of u_h and u^* . The pair (u_h, u^*) satisfies the non-standard transmission problem

$$\begin{cases} \Delta u^* - s^2 u^* = 0, & \text{in } \mathbb{R}^d \setminus \Gamma, \\ [\partial_\nu u^*] \in X_h, \\ [\gamma u^*] - \gamma u_h = d_3, \quad X_h^t \gamma^- u^* = d_2, \\ A_{\Omega_-}^h(s)u_h + \gamma_h^+ \partial_\nu^+ u^* = d_1, \end{cases}$$

where $(d_1, d_2, d_3) \in V'_h \times X'_h \times Y_d$. Not surprisingly this problem is very similar to problem (45) with the condition on the jump $[\gamma u^*]$ relaxed. We can find a weak formulation of this problem in the space $V_h \times H^1(\mathbb{R}^d \setminus \Gamma)$. The remainder of the proof follows the same steps as in previous examples.

8 Homogeneous obstacles

We now go back to the transmission problem (32) and assume that both interior coefficients are constant. To simplify we write $\alpha = \kappa_0$ and $c^{-2} = \kappa_1/\kappa_0$. The equations in frequency domain are:

$$\begin{cases} \Delta u - (s/c)^2 u = 0, & \text{in } \Omega_-, \\ [\gamma u] = \gamma u_{inc}, & \text{on } \Gamma, \\ \alpha \partial_\nu^- u - \partial_\nu^+ u = \partial_\nu u_{inc}, & \text{on } \Gamma, \\ \Delta u - s^2 u = 0, & \text{in } \Omega_+. \end{cases} \tag{46}$$

In this case both the interior and exterior fields can be represented from the boundary. We are going to follow here the method of Costabel and Stephan [11]. The symmetric method of [22] is also applicable but we will not present the details here. The unknowns for the coupled system will be

$$\lambda := \partial_\nu^- u, \quad \phi := \gamma^- u.$$

Green’s Third Theorem allows us to represent the solution as

$$u = \begin{cases} S(s/c)\lambda - D(s/c)\phi, & \text{in } \Omega_-, \\ -S(s)(\alpha\lambda - \partial_\nu u_{inc}) + D(s)(\phi - \gamma u_{inc}), & \text{in } \Omega_+. \end{cases} \tag{47}$$

The jump conditions of potentials applied to (47) and the transmission conditions in (46) give the following integral system

$$\begin{aligned} & \begin{bmatrix} V(s/c) + \alpha V(s) & -K(s/c) - K(s) \\ K^t(s/c) + K^t(s) & W(s/c) + \alpha^{-1}W(s) \end{bmatrix} \begin{bmatrix} \lambda \\ \phi \end{bmatrix} \\ &= \begin{bmatrix} V(s) & \frac{1}{2}I - K(s) \\ \alpha^{-1}(\frac{1}{2}I + K^t(s)) & \alpha^{-1}W(s) \end{bmatrix} \begin{bmatrix} \partial_\nu u_{\text{inc}} \\ \gamma u_{\text{inc}} \end{bmatrix}. \end{aligned} \tag{48}$$

As in previous examples we will copy the data in two variables to deal both with how they are affected by integral operators and with the possibility of discretizing them in space. Therefore we need four closed spaces, two for unknowns (subscripted with u) and two for data (subscripted with d):

$$X_u, X_d \subset H^{-1/2}(\Gamma), \quad Y_u, Y_d \subset H^{1/2}(\Gamma).$$

As in Sect. 5, we consider two matrices of operators to represent both sides of (48)

$$\begin{aligned} \mathbf{H}_1(s) &:= \begin{bmatrix} X'_u & 0 \\ 0 & Y'_u \end{bmatrix} \begin{bmatrix} V(s/c) + \alpha V(s) & -K(s/c) - K(s) \\ K^t(s/c) + K^t(s) & W(s/c) + \alpha^{-1}W(s) \end{bmatrix} \begin{bmatrix} X_u & 0 \\ 0 & Y_u \end{bmatrix} \\ \mathbf{H}_2(s) &:= \begin{bmatrix} X'_u & 0 \\ 0 & Y'_u \end{bmatrix} \begin{bmatrix} V(s) & \frac{1}{2}I - K(s) \\ \alpha^{-1}(\frac{1}{2}I + K^t(s)) & \alpha^{-1}W(s) \end{bmatrix} \begin{bmatrix} X_d & 0 \\ 0 & Y_d \end{bmatrix}. \end{aligned}$$

The full system is described by a single operator acting from $X_u \times Y_u \times X_d \times Y_d$ into $X'_u \times Y'_u \times X_d \times Y_d$

$$\mathbf{H}_{\text{CS}}(s) \begin{bmatrix} \lambda \\ \phi \\ \lambda_d \\ \phi_d \end{bmatrix} := \begin{bmatrix} \mathbf{H}_1(s) & -\mathbf{H}_2(s) \\ 0 & \mathbf{I} \end{bmatrix} \begin{bmatrix} \lambda \\ \phi \\ \lambda_d \\ \phi_d \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \end{bmatrix}. \tag{49}$$

We will take one of the following three choices:

- (a) All of the subspaces are taken to be the full space. This case corresponds to the exact continuous operator. The right-hand side that makes this system equivalent to (48) is simply $(0, 0, \partial_\nu u_{\text{inc}}, \gamma u_{\text{inc}})$.
- (b) $X_u = X_h$ and $Y_u = Y_h$ are finite-dimensional spaces and X_d and Y_d are left as before. This case corresponds to a traditional Galerkin discretization of the Eq. (48).
- (c) X_u and Y_u are as in (b) but now $X_d = X_d^h$ and $Y_d = Y_d^h$ are finite-dimensional too. This case corresponds to the preprocessing of data in a discrete space plus the Galerkin discretization of (48). Section 5 shows how this process is carried out.

Before proceeding any further, let us remark that the type of transmission conditions that are going to appear in the non-standard transmission problem can be guessed by trying to reconstruct the matrix of integral operators from the potential expression (47). In fact, it is simple to prove that

$$\begin{bmatrix} \gamma^+ & \gamma^- \\ \alpha^{-1} \partial_v^+ & \partial_v^- \end{bmatrix} \begin{bmatrix} S(s/c) & -D(s/c) & 0 & 0 \\ \alpha S(s) & -D(s) & -S(s) & D(s) \end{bmatrix} = [\mathbf{H}_1(s) \quad -\mathbf{H}_2(s)]$$

The left-most matrix gives the conditions that will be imposed, whereas the matrix of potentials is the one relating the integral system with the transmission problem.

Proposition 11 *The operator $\mathbf{H}_{CS}(s)$ is invertible for all $s \in \mathbb{C}_+$ and*

$$\mathbf{H}_{CS}^{-1} \in \mathcal{A} \left(\frac{5}{2}, X'_u \times Y'_u \times X_d \times Y_d, X_u \times Y_u \times X_d \times Y_d \right).$$

All constants in the bounds can be taken independent of the choice of the spaces. In the discrete case we thus have elements of the uniform classes. Finally the operator

$$\begin{bmatrix} S(s/c) & -D(s/c) & 0 & 0 \\ \alpha S(s) & -D(s) & -S(s) & D(s) \end{bmatrix} \mathbf{H}_{CS}^{-1}(s) \tag{50}$$

belongs to $\mathcal{A}(2, X'_u \times Y'_u \times X_d \times Y_d, H^1(\Omega_-) \times H^1(\Omega_+))$ with constants independent of the choice of the spaces.

Proof First step. Problem (49) is equivalent to the system of transmission problems

$$\begin{cases} \Delta u - s^2 u = 0, & \text{in } \mathbb{R}^d \setminus \Gamma, \\ \Delta u^* - (s/c)^2 u^* = 0, & \text{in } \mathbb{R}^d \setminus \Gamma, \\ [\gamma u] \in Y_u, \quad [\partial_v u] \in X_u, \\ [\gamma u] - [\gamma u^*] = d_4, \quad \alpha [\partial_v u] - [\partial_v u^*] = d_3, \\ X_u^t (\gamma^+ u + \gamma^- u^*) = d_1, \quad Y_u^t (\alpha \partial_v^- u + \partial_v^+ u^*) = \alpha d_2, \end{cases} \tag{51}$$

as follows: given a solution to (49), the pair

$$u := S(s/c)\lambda - D(s/c)\phi, \quad u^* := S(s)(\alpha\lambda - \lambda_d) - D(s)(\phi - \phi_d)$$

solves (51), and reciprocally $([\partial_v u], [\gamma u], d_3, d_4)$ provides a solution to (49).

Second step. Let us now find a weak formulation for (51). The main space is

$$\widehat{H} := \left\{ (u, u^*) \in H^1(\mathbb{R}^d \setminus \Gamma) \times H^1(\mathbb{R}^d \setminus \Gamma) \mid [\gamma u] \in Y_u \right\},$$

the generalized trace operator associates

$$\widehat{H} \ni (u, u^*) \mapsto \widehat{\gamma}(u, u^*) := (X_u^t (\gamma^+ u + \gamma^- u^*), [\gamma u] - [\gamma u^*]) \in X'_u \times H^{1/2}(\Gamma)$$

and its kernel is

$$\widehat{H}_0 := \left\{ (v, v^*) \in H^1(\mathbb{R}^d \setminus \Gamma) \times H^1(\mathbb{R}^d \setminus \Gamma) \mid \begin{aligned} &\gamma^+ v + \gamma^- v^* \in X_u^o, \\ &[\gamma v] = [\gamma v^*] \in Y_u \end{aligned} \right\}.$$

Then (51) is equivalent to

$$\left[\begin{aligned} &(u, u^*) \in \widehat{H}, \quad \widehat{\gamma}(u, u^*) = (d_1, d_4), \\ &\alpha \langle A_{\mathbb{R}^d \setminus \Gamma}(s/c)u, v \rangle + \langle A_{\mathbb{R}^d \setminus \Gamma}(s)u^*, v^* \rangle = \alpha \langle d_2, [\gamma v] \rangle - \langle d_3, \gamma^- v^* \rangle, \\ &\forall (v, v^*) \in \widehat{H}_0. \end{aligned} \right] \quad (52)$$

The proof of this assertion can be verified by following carefully the technique explained in the previous sections. Let us just show what the key points are in a very condensed form. First of all we have the identity for arbitrary $(v, v^*) \in \widehat{H}_0$

$$\begin{aligned} &\alpha (\langle \partial_v^- u, \gamma^- v \rangle - \langle \partial_v^+ u, \gamma^+ v \rangle) + \langle \partial_v^- u^*, \gamma^- v^* \rangle - \langle \partial_v^+ u^*, \gamma^+ v^* \rangle \\ &= \langle \alpha \partial_v^- u + \partial_v^+ u^*, [\gamma v] \rangle + \alpha \langle [\partial_v u], \gamma^+ v + \gamma^- v^* \rangle - \langle \alpha [\partial_v u] - [\partial_v u^*], \gamma^- v^* \rangle. \end{aligned}$$

The second point is the realization that the three types of boundary values in the right-hand side of the preceding identity

$$[\gamma v^*] = [\gamma v] \in Y_u, \quad \gamma^+ v + \gamma^- v^* \in X_u^o, \quad \gamma^- v^* \in H^{1/2}(\Gamma)$$

can be chosen independently. With these ideas, it is simple to prove the equivalence of both problems.

Third step. We have to find a right-inverse of $\widehat{\gamma}$ with norm independent of the choice of the spaces. Because the liftings of the trace can be done independently for the interior and exterior domains, if we want to fix values of

$$\gamma^+ u + \gamma^- u^* = \xi_1, \quad [\gamma u] - [\gamma u^*] = \xi_2$$

demanding that $[\gamma u] \in Y_u$, the simplest choice is to pick

$$\gamma^- u = \gamma^+ u = \gamma^- u^* = \xi_1/2, \quad \gamma^+ u^* = \xi_2 + \xi_1/2$$

so that we do not even have to worry about the restriction on the jump of the trace of u , which is set to zero. In fact, we need to impose the value of $X_u^t(\gamma^+ u + \gamma^- u^*)$, but as usual, we first extend the given functional in X'_u to another one in $H^{-1/2}(\Gamma) = H^{-1/2}(\Gamma)'$ with the same norm.

The *fourth step* and the bounds for the potential postprocessing do not differ from what we have already done several times. □

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Appendix 1: Convolution quadrature

There are two families of convolution quadrature (CQ) methods. One is related to multistep methods and can be considered as a scalar valued method. The second one is related to Runge–Kutta methods and can be considered as a vector-valued scheme.

In general we can assume that our problem is of the following abstract form: given d , solve

$$f_1 * g = d \tag{53}$$

and then postprocess to compute

$$u = f_2 * g. \tag{54}$$

All elements participating in these expressions are functions of the time variable beginning at $t = 0$. In fact behavior with respect to the time variable can be distributional (as will be the case for all of our examples). It helps to imagine that f_1 and f_2 are matrix-valued and g is vector valued. In truth, both f_1 and f_2 will be operator-valued and g will take values on a function space.

Convolution quadrature works with the Laplace transform of the convolution operators f_1 and f_2 , but uses the data function d in time and provides approximations of g and u in time too. The respective Laplace transforms of f_1 and f_2 will be denoted F_1 and F_2 . Some basic assumptions on f_1 and f_2 (actually on their Laplace transforms) are given in Sect. 2.

For the moment we perform all the manipulations formally. Note that the double process of solving and postprocessing can be seen as a single system of equations:

$$\begin{bmatrix} f_1 & 0 \\ f_2 & -\delta_0 \end{bmatrix} * \begin{bmatrix} g \\ u \end{bmatrix} = \begin{bmatrix} d \\ 0 \end{bmatrix}, \tag{55}$$

where convolution with the Dirac delta at zero is the identity operator (properly speaking we should write $\delta_0 \otimes I$, where I is the identity operator in the space where u takes values). In the frequency domain the operator associated to these equations is

$$\begin{bmatrix} F_1(s) & 0 \\ F_2(s) & -I \end{bmatrix}. \tag{56}$$

Its inverse is

$$\begin{bmatrix} F_1^{-1}(s) & 0 \\ F_2(s)F_1^{-1}(s) & -I \end{bmatrix}$$

so we will have to pay attention to both F_1^{-1} and $F_2F_1^{-1}$.

The derivation of the method can be found in [25] for the multistep-based method and in [29] for the Runge–Kutta (RK) case. We remark that the use of the RK-based

methods for scattering problems has still to be explored. We are just going to explain here the scalar-valued schemes, associated to multistep methods. For RK-based methods, we refer the reader to the original article [29], to the more recent [5] and, in the context of waves and integral equations, to [23].

The method uses a fixed time-step $k > 0$ and works on the uniform grid

$$t_n := nk, \quad n \geq 0.$$

Let us first deal with the problem still written in form (53), (54). The main ingredient of the method is a scalar complex function p such that:

- (a) It is holomorphic in a disk centered at the origin with radius $r > 1$.
- (b) $\text{Re } p(\zeta) > 0$ for all $|\zeta| < 1$.
- (c) There exists $q \geq 1$ such that

$$h^{-1} p(e^{-h}) = 1 + \mathcal{O}(h^q), \quad \text{as } h \rightarrow 0^+.$$

Note that (c) implies the existence of a simple zero of p at $\zeta = 1$.

The second ingredient of the method consists of the derivation of two power expansions

$$F_j(p(\zeta)/k) = \sum_{n=0}^{\infty} \omega_n^j(k) \zeta^n, \quad j = 1, 2.$$

Hypothesis (b) together with the requirement that $F_j \in \mathcal{A}(\mu, X, Y)$ for some μ , guarantee that this expansion can be done. In this paper we assumed that the weight coefficients are computed exactly. Note that when working with acoustic waves, apart from the possibility of using contour integrals as in [17, 21] or [36] the corresponding operators of the expansion can be dealt with exactly [23]. For the moment being, it is enough to assume that we can compute exactly $\omega_n^j(k)$ for all the operators involved.

We can now apply the method. The convolution equation (53) is translated into the triangular process

$$\omega_0^1(k)g_n = d(t_n) - \sum_{m=1}^n \omega_m^1(k)g_{n-m}$$

that computes progressively values $g_n \approx g(t_n)$. The postprocess (54) keeps the same causal relation that the discrete convolution equation does and approximates

$$u(t_n) \approx \sum_{m=0}^n \omega_m^2(k)g_{n-m}.$$

Note that we do not have to wait for the full sequence of g_n to be computed to begin the postprocess. It is simple to see that if we apply the process directly to the convolution equation (55), the expansion associated to (56) is just

$$\sum_{n=0}^{\infty} \begin{bmatrix} \omega_n^1(k) & 0 \\ \omega_n^2(k) & \delta_{n,0} \end{bmatrix} \zeta^n,$$

($\delta_{n,0}$ is the Kronecker symbol) and we end up with exactly the same numerical scheme. Therefore, we can restrict our attention to convolution equations and consider post-processing as part of a wider equation.

The simplest examples are the methods derived from the backward Euler scheme and from BDF2

$$1 - \zeta, \quad \frac{3}{2} - 2\zeta + \frac{1}{2}\zeta^2,$$

with respective values of q equalling one and two. Unfortunately, it is known since long time ago that it is impossible to obtain $q = 3$ or higher in hypothesis (c) preserving hypothesis (b) if p is rational. In the numerical ODE community this result is known as the second Dahlquist barrier and states that there are no A-stable multistep methods of order larger than two (see [18, Chapter V]). For higher order we can always revert to the RK-based methods. When p is rational, we can easily prove the following result, using the CQ discrete operator calculus, or a purely mechanical manipulation of discrete convolutions.

Proposition 12 *Assume that p is a rational function and let us write*

$$p(\zeta)^2 = \frac{q_0 + q_1\zeta + \dots + q_N\zeta^N}{r_0 + r_1\zeta + \dots + r_N\zeta^N}.$$

Consider operators of the form $F_1(s) = A_0 + s^2A_1 + B(s)P$ and expand

$$B(p(\zeta)/k) = \sum_{n=0}^{\infty} \omega_n^b(k)\zeta^n.$$

*Then the CQ method applied to $f_1 * g = d$ is equivalent to the combined recurrence*

$$\begin{aligned} (r_0A_0 + k^{-2}q_0A_1)g_n + r_0\lambda_n &= \sum_{m=0}^{\min\{N,n\}} r_m d(t_{n-m}) \\ &\quad - \sum_{m=1}^{\min\{N,n\}} \left((r_mA_0 + k^{-2}q_mA_1)g_{n-m} + r_m\lambda_{n-m} \right) \\ \omega_0^b(k)Pg_n - \lambda_n &= \sum_{m=1}^n \omega_m^b(k)\rho_{n-m} \end{aligned}$$

where $\rho_n := Pg_n$.

When $A_0 = 0, A_1 = I, B(s) \equiv 0$, we recover the multistep method to the differential equation $u'' = \delta_0'' * u = d$ with zero initial conditions. The meaning of the

recurrence is the following: the explicit occurrences of the unknown g_n include only a finite number of memory terms, as in a multistep method, whereas the long-term memory is handled by the auxiliary variable λ_n which only uses $\rho_n = P g_n$ in the past times.

In the example of Sect. 6, $P(u, \lambda, \phi) = (\lambda, \phi)$ and only the variables on the boundary have to be retained for all past times, whereas the unknown in the interior is kept as long as the multistep method uses it. This means that the time discretization of the system in this section is a multistep-type discretization of a differential equation with non-standard boundary conditions that require memory and proceeds from a CQ-discretization of an integral form of the exterior Dirichlet-to-Neumann operator (the one in Sect. 4). We can therefore understand the whole scheme as a time-stepping method with absorbing boundary conditions.

In the example of Sect. 7, $P(u, \lambda) := (\gamma u, \lambda)$ and we only have to retain the boundary unknown λ and the trace of the interior unknown.

Sometimes we will find that instead of (53) we have an equation of the kind

$$f_1 * g = f_3 * d,$$

i.e., data are also affected by a convolution operator. The treatment of this equation is similar and can be put in the same frame of convolution equations by copying data as an additional unknown

$$\begin{bmatrix} f_1 & -f_3 \\ 0 & \delta_0 \end{bmatrix} * \begin{bmatrix} g \\ g_d \end{bmatrix} = \begin{bmatrix} 0 \\ d \end{bmatrix}.$$

The value of μ in Sect. 2 (and in all our examples) is relevant in imposing regularity conditions for data in CQ to restore full order of convergence in the time variable (see [27, Theorems 3.1–3.3]). For instance, a specialization of Theorem 3.2 in [27] reads as follows:

Proposition 13 *Assume that p satisfies the hypotheses above and that $F \in \mathcal{A}(\mu, X, Y)$. Let $u := f * g$ and let $u_n \approx u(t_n)$ be the p -based CQ approximation of u at the discrete time $t_n := nk$. If*

$$g \in H^m((0, T), X), \quad g(0) = \dots = g^{(m-1)}(0) = 0$$

with $m > \mu + q + \frac{1}{2}$, then

$$\|u(t) - u_n\| \leq C(T)k^q \left(\int_0^T |g^{(m)}(t)|^2 dt \right)^{1/2},$$

for all $t_n \leq T$.

For the only result on time-and-space discretization that we are aware of, see [27, Theorem 5.4]: once full order of discretization is attained in the time variable, error

caused by the space discretization follows from analysis of stable Galerkin methods and careful arguments on best approximation in Sobolev spaces.

Appendix 2: Operators associated to $\Delta - s^2$

2.1 Formulas

For easy reference we list here several useful formulas related to potentials, boundary integral operators and Steklov–Poincaré type operators. All formulas hold for any value of s , so we are free to write some of them as formulas satisfied by analytic functions of the parameter s . The following formulas are known as the *jump relations* of potentials:

$$\gamma^\pm S = V, \quad \partial_\nu^\pm S = \mp \frac{1}{2}I + K^t, \quad \gamma^\pm D = \pm \frac{1}{2}I + K, \quad \partial_\nu^\pm D = -W. \tag{57}$$

The Dirichlet-to-Neumann (Steklov–Poincaré) operators and their inverses admit several different expressions in terms of the boundary integral operators. Note that since $DtN^{-1} = NtD$ each of them gives another one using inverses:

$$\begin{aligned} DtN^- &= V^{-1} \left(\frac{1}{2}I + K \right) &= \left(\frac{1}{2}I + K \right)^t V^{-1} = W + \left(\frac{1}{2}I + K \right)^t V^{-1} \left(\frac{1}{2}I + K \right), \\ -DtN^+ &= V^{-1} \left(\frac{1}{2}I - K \right) &= \left(\frac{1}{2}I - K \right)^t V^{-1} = W + \left(\frac{1}{2}I - K \right)^t V^{-1} \left(\frac{1}{2}I - K \right), \\ NtD^- &= W^{-1} \left(\frac{1}{2}I - K \right)^t &= \left(\frac{1}{2}I - K \right) W^{-1} = V + \left(\frac{1}{2}I - K \right)^t W^{-1} \left(\frac{1}{2}I - K \right)^t, \\ -NtD^+ &= W^{-1} \left(\frac{1}{2}I + K \right)^t &= \left(\frac{1}{2}I + K \right) W^{-1} = V + \left(\frac{1}{2}I + K \right)^t W^{-1} \left(\frac{1}{2}I + K \right)^t. \end{aligned} \tag{58}$$

In particular, adding two consecutive equations in (58) we obtain

$$V^{-1} = DtN^- - DtN^+, \quad W^{-1} = NtD^- - NtD^+. \tag{59}$$

Any solution to $\Delta u - s^2 u = 0$ in $\mathbb{R}^d \setminus \Gamma$ can be written as $u = S(s)[\partial_\nu u] - D(s)[\gamma u]$. Taking u to be identically zero in Ω_- , we have the formulas satisfied for exterior solutions

$$u = D(s)\gamma^+ u - S(s)\partial_\nu^+ u, \quad \begin{bmatrix} V(s) & \frac{1}{2}I - K(s) \\ \left(\frac{1}{2}I + K(s) \right)^t & W(s) \end{bmatrix} \begin{bmatrix} \partial_\nu^+ u \\ \gamma^+ u \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{60}$$

2.2 Bounds

The first important result in this section is a Lemma from [2].

Lemma 14 *Let \mathcal{O} be a bounded open set with Lipschitz boundary or the exterior of one of such sets. Then there exists $C_{\mathcal{O}}$ such that for any $\delta > 0$ and $\phi \in H^{1/2}(\partial\mathcal{O})$, the solution of*

$$\begin{cases} -\Delta u + \delta^2 u = 0, & \text{in } \mathcal{O}, \\ u = \phi, & \text{on } \partial\mathcal{O}, \end{cases} \tag{61}$$

satisfies

$$\|u\|_{\delta, \mathcal{O}} \leq C_{\mathcal{O}} \max\{1, \delta\}^{1/2} \|\phi\|_{1/2, \partial\mathcal{O}}. \tag{62}$$

The result can be stated also as the existence of a family of liftings of the trace operator, depending on the parameter δ such that (62) holds taking u as such lifting. Note that the solution to (61) is the function in $H^1(\mathcal{O})$ such that its trace is ϕ and its $\|\cdot\|_{\delta, \mathcal{O}}$ norm is minimal. A bound similar to (62) but with δ in place of $\delta^{1/2}$ is straightforward to prove.

The proof of Lemma 14 is given in [2] by using local charts. Note that the result in [2] is proved for smooth boundaries but that Lipschitz regularity is enough for the arguments to hold. Note also that the corresponding Lemma in [2] uses a certain complex parameter instead of the positive real number δ . Our statement is a particular case of that one but the general case is a consequence of the particular case, so this result is as general as the original. Finally, when comparing results in this section with those of [2], one has to be careful to translate the variable s to $i\omega$: following the French tradition (see [13]), the Laplace transform is rotated ninety degrees in the complex plane; it is just an extension of the Fourier transform with the aim of applying directly the Payley–Wiener theorems.

Lemma 15 *Let \mathcal{O} be as in Lemma 14 and $C_{\mathcal{O}}$ be the constant of the inequality (62). Given $u \in H^1(\mathcal{O})$ such that $\Delta u - s^2 u = 0$ we have*

$$\|\partial_v u\|_{-1/2, \partial\mathcal{O}} \leq C_{\mathcal{O}} \left(\frac{|s|}{\sigma}\right)^{1/2} \|u\|_{|s|, \mathcal{O}}.$$

Proof Let $\phi \in H^{1/2}(\partial\mathcal{O})$ and take v as in (61). Then by (6) and (62) it follows that

$$\begin{aligned} |\langle \partial_v u, \phi \rangle| &= \left| \int_{\mathcal{O}} \nabla u \cdot \nabla v + s^2 \int_{\mathcal{O}} u v \right| = |\langle A_{\mathcal{O}}(s)u, v \rangle| \\ &\leq \|u\|_{|s|, \mathcal{O}} \|v\|_{|s|, \mathcal{O}} \leq C_{\mathcal{O}} \max\{1, |s|^{1/2}\} \|\phi\|_{1/2, \partial\mathcal{O}} \|u\|_{|s|, \mathcal{O}} \\ &\leq C_{\mathcal{O}} \frac{|s|^{1/2}}{\sigma^{1/2}} \|\phi\|_{1/2, \partial\mathcal{O}} \|u\|_{|s|, \mathcal{O}}. \end{aligned}$$

The result is a simple consequence of the definition of the $H^{-1/2}(\partial\mathcal{O})$ norm. □

From here on we revert to the geometrical setting of Sect. 4: Ω_- and Ω_+ are separated by a closed Lipschitz interface Γ . By applying Lemma 15 to Ω_- and Ω_+ we can easily prove that if $\Delta u - s^2 u = 0$ in $\mathbb{R}^d \setminus \Gamma = \Omega_- \cup \Omega_+$, then

$$\|[\partial_v u]\|_{-1/2, \Gamma} \leq C \frac{|s|^{1/2}}{\sigma^{1/2}} \|u\|_{|s|, \mathbb{R}^d \setminus \Gamma}. \tag{63}$$

We now begin to prove the bounds given in the tables of Sect. 4. Note that every time we obtain an ellipticity result we have a bound for the inverse operator by Proposition 3. The ellipticity bounds for V in Proposition 16 and W in Proposition 19 appear already in [2, 3].

Proposition 16 *The single-layer potential satisfies $S \in \mathcal{A}(1, H^{-1/2}(\Gamma), H^1(\mathbb{R}^d))$. The corresponding boundary operator satisfies*

$$V \in \mathcal{E}\left(2, \text{Arg}, H^{-1/2}(\Gamma)\right) \cap \mathcal{A}\left(1, H^{-1/2}(\Gamma), H^{1/2}(\Gamma)\right).$$

Proof Let $\lambda \in H^{-1/2}(\Gamma)$ and $u := S(s)\lambda$, so that $\lambda = [\partial_\nu u]$ and $\gamma u = V(s)\lambda$. Then

$$\langle \bar{\lambda}, V(s)\lambda \rangle = \langle A_{\mathbb{R}^d \setminus \Gamma}(\bar{s})u, \bar{u} \rangle.$$

Hence by (7) and (63)

$$\text{Re}\left(e^{i \text{Arg } s} \langle \bar{\lambda}, V(s)\lambda \rangle\right) = \frac{\sigma}{|s|} \|u\|_{|s|, \mathbb{R}^d \setminus \Gamma}^2 \geq C \frac{\sigma}{|s|^2} \|\lambda\|_{-1/2, \Gamma}^2,$$

which proves the desired ellipticity estimate. On the other hand by (5)

$$\begin{aligned} \frac{\sigma}{|s|} \frac{\sigma^2}{|s|} \|u\|_{1, \mathbb{R}^d \setminus \Gamma}^2 &\leq \frac{\sigma}{|s|} \|u\|_{|s|, \mathbb{R}^d \setminus \Gamma}^2 \leq |\langle \bar{\lambda}, V(s)\lambda \rangle| = |\langle \bar{\lambda}, \gamma u \rangle| \\ &\leq \|\gamma u\|_{1/2, \Gamma} \|\lambda\|_{-1/2, \Gamma} \leq C \|u\|_{1, \mathbb{R}^d \setminus \Gamma} \|\lambda\|_{-1/2, \Gamma}, \end{aligned}$$

where C is the continuity constant for the trace theorem. This gives the estimate for $S(s)$. Given the fact that $V(s) = \gamma S(s)$ the remaining assertion follows readily. \square

Proposition 17 $\text{DtN}^-, -\text{DtN}^+, V^{-1} \in \mathcal{E}(1, -\text{Arg}, H^{1/2}(\Gamma))$.

Proof Let $\phi \in H^{1/2}(\Gamma)$ and define u as the solution to

$$\begin{cases} \Delta u - s^2 u = 0, & \text{in } \Omega_-, \\ \gamma u = \phi, & \text{on } \Gamma, \end{cases}$$

so that $\partial_\nu u = \text{DtN}^-(s)\phi$. Then $\langle A_{\Omega_-}(s)u, \bar{u} \rangle = \langle \text{DtN}^-(s)\phi, \bar{\phi} \rangle$ and hence by (7), (5) and the trace theorem

$$\text{Re}\left(e^{-i \text{Arg } s} \langle \text{DtN}^-(s)\phi, \bar{\phi} \rangle\right) = \frac{\sigma}{|s|} \|u\|_{|s|, \Omega_-}^2 \geq \frac{\sigma}{|s|} \|u\|_{1, \Omega_-}^2 \geq C \frac{\sigma}{|s|} \|\phi\|_{1/2, \Gamma}^2.$$

A similar bound can be easily obtained for $-\text{DtN}^+$ (note that the change of sign is due to the reorientation of the normal vector which now points inwards). Finally, by the first identity of (59) and since $\mathcal{E}(1, -\text{Arg}, H^{-1/2}(\Gamma))$ is a vector space, V^{-1} belongs to this space. Note that this result gives an alternative proof to the fact that $V \in \mathcal{A}(1, H^{-1/2}(\Gamma), H^{1/2}(\Gamma))$ (see Proposition 16). \square

Proposition 18 $\text{NtD}^-, -\text{NtD}^+, W^{-1} \in \mathcal{E}(2, \text{Arg}, H^{-1/2}(\Gamma))$.

Proof Let $\lambda \in H^{-1/2}(\Gamma)$ and define u as the solution to

$$\begin{cases} \Delta u - s^2 u = 0, & \text{in } \Omega_-, \\ \partial_\nu u = \lambda, & \text{on } \Gamma, \end{cases}$$

so that $\gamma u = \text{NtD}^{-1}(s)u$. Then, using again (7) and Lemma 15 it follows that

$$\begin{aligned} \text{Re} \left(e^{i \text{Arg}s} \langle \bar{\lambda}, \text{NtD}^-(s)\lambda \rangle \right) &= \text{Re} \left(e^{i \text{Arg}s} A_{\Omega_-}(\bar{s})u, \bar{u} \right) = \frac{\sigma}{|s|} \|u\|_{|s|, \Omega_-}^2 \\ &\geq \frac{\sigma}{|s|^2} \|\lambda\|_{-1/2, \Gamma}^2. \end{aligned}$$

The proof for NtD^+ is very similar and the second identity in (59) proves the remaining bound. □

Proposition 19 *The double-layer potential satisfies $D \in \mathcal{A}(\frac{3}{2}, H^{1/2}(\Gamma), H^1(\mathbb{R}^d \setminus \Gamma))$ and the hypersingular operator satisfies $W \in \mathcal{E}(1, -\text{Arg}, H^{1/2}(\Gamma))$.*

Proof Let $\phi \in H^{1/2}(\Gamma)$ and define $u := -D(s)\phi$, so that $[\gamma u] = \phi$ and $\partial_\nu^\pm u = W(s)\phi$ and

$$\langle W(s)\phi, \bar{\phi} \rangle = \langle A_{\mathbb{R}^d \setminus \Gamma}(s)u, \bar{u} \rangle.$$

Using the same arguments of preceding propositions we easily prove that

$$\text{Re} \left(e^{-i \text{Arg}s} \langle W(s)\phi, \bar{\phi} \rangle \right) = \frac{\sigma}{|s|} \|u\|_{|s|, \mathbb{R}^d \setminus \Gamma}^2 \geq \frac{\sigma \sigma^2}{|s|} \|u\|_{1, \mathbb{R}^d \setminus \Gamma}^2 \geq C_\Gamma \frac{\sigma \sigma^2}{|s|} \|\phi\|_{1/2, \Gamma}^2,$$

as well as

$$\frac{\sigma}{|s|} \|u\|_{|s|, \mathbb{R}^d \setminus \Gamma}^2 \leq |\langle W(s)\phi, \bar{\phi} \rangle| \leq \|W(s)\phi\|_{-1/2, \Gamma} \|\phi\|_{1/2, \Gamma} \leq C \frac{|s|^2}{\sigma \underline{\sigma}} \|\phi\|_{1/2, \Gamma}^2,$$

where in the last step we have used the boundedness property of $W(s)$ that is derived from the ellipticity of $W^{-1}(s)$ (Proposition 18). The previous inequalities prove the statement. □

Proposition 20 $K \in \mathcal{A}(\frac{3}{2}, H^{1/2}(\Gamma), H^{1/2}(\Gamma))$ and $K^t \in \mathcal{A}(\frac{3}{2}, H^{-1/2}(\Gamma), H^{-1/2}(\Gamma))$.

Proof Note that $\frac{1}{2}I + K(s) = \gamma^+ D(s)$. Applying then Proposition 19 and the fact that $I \in \mathcal{A}(0, H^{1/2}(\Gamma), H^{1/2}(\Gamma))$ we obtain the result for K . The one for K^t is obtained by transposition. □

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