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Characterizing inclusions in optical tomography

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Abstract
In optical tomography, one tries to determine the spatial absorption and scattering distributions inside a body by using measured pairs of inward and outward fluxes of near-infrared light on the object boundary. In many practically important situations, the scatter and the absorption inside the object are smooth apart from inclusions where at least one of the two optical parameters jumps to a higher or lower value. In this work, we investigate the possibility of characterizing these inhomogeneities in the framework of the diffusion approximation of the radiative transfer equation using the factorization method: for purely scattering inclusions, or if the scattering and absorption coefficients interplay in a correct way, the outcoming flux corresponding to a point source belongs to the range of an operator, determined through boundary measurements, if and only if the point source lies inside one of the inclusions.

1. Introduction

In optical tomography, a physical body is illuminated with a flux of near-infrared (NIR) photons and the outcoming flux is measured on the surface of the body. The idea is to reconstruct the optical properties inside the object by using the measured pairs of input and output fluxes. NIR tomography has a few possible clinical applications, the most important of which are, arguably, screening for breast cancer and the development of a cerebral imaging modality for mapping structure and function in newborn infants, and also possibly adults. For more medical and instrumental details we refer to [1–3, 7] and the references therein.

In the framework of transport theory, propagation of light in tissue is modelled by the radiative transport equation (RTE). Since a straight application of RTE is numerically quite expensive, the model is usually simplified by using the diffusion approximation, which is well established for materials that are strongly scattering [1]. If it is assumed that the flux conducted through the object boundary is either static in time or modulated with a fixed harmonic frequency, the diffusion approximation of RTE leads to an elliptic partial differential equation, the coefficients of which are what one needs to reconstruct when solving the inverse problem of optical tomography.

In this work, we consider the situation where the background optical properties of the investigated object are known but the object is contaminated with a number of inhomogeneities with unknown characteristics. We investigate the possibility of characterizing these inclusions using the factorization method introduced and justified for inverse scattering in [11], and later for electrical impedance tomography with classical boundary conditions in [4] and with complete electrode boundary conditions in [10]. Our aim is to derive sufficient conditions for the factorization procedure to be functional in the framework of the diffusion approximation.

This text is organized as follows. Section 2 introduces the radiative transfer equation and its diffusion approximation. In section 3, we consider briefly the unique solvability of the forward model associated with the diffusion approximation and introduce the Robin-to-Robin boundary operator that maps the used input flux onto the measured output flux. The factorization of the difference of two Robin-to-Robin maps, one corresponding to the background optical properties and the other corresponding to the object with inclusions, is conducted in section 4. Section 5 investigates the properties of the operators needed in the factorization, and finally in section 6 we state the characterization results.

2. Approximating light propagation

Propagation of electromagnetic radiation in a medium is governed by Maxwell's equations. Particularly, this holds for our case of interest, namely, near-infrared light travelling through some biological tissue. However, since the wavelength of NIR light is small compared to the characteristic distances of human tissue, the exact models are totally useless. Therefore, we will model light propagation by using the diffusion approximation of the radiative transfer equation, which has been shown to model fairly well light propagation in strongly scattering tissues.

2.1. Radiative transfer equation

Let $\Omega \subset \mathbb{R}^n, n = 2$ or $n = 3$ be a bounded body with a smooth boundary and connected complement. The radiance at $x \in \Omega$ at time $t \in \mathbb{R}$ in direction $\hat{\theta} \in S^{n-1}$ is written as $I(x, t, \hat{\theta})$. In the framework of transport theory, this scalar function satisfies the radiative transfer equation,

$$\begin{aligned}\frac{1}{c} I_t(x, t, \hat{\theta}) + \hat{\theta} \cdot \nabla I(x, t, \hat{\theta}) + (\mu(x) + \mu_s(x)) I(x, t, \hat{\theta})\\ - \mu_s(x) \int_{S^{n-1}} f(x, \hat{\theta}, \hat{\omega}) I(x, t, \hat{\omega}) \, \mathrm{d}s(\hat{\omega}) = q(x, t, \hat{\theta}),\end{aligned} \tag{2.1}$$

where c is the speed of light (assumed to be constant), the positive scalar functions μ and μ_s are the absorption and scattering coefficients, respectively and q denotes the source term which is assumed to vanish in this discussion. The kernel f is the scattering phase function, satisfying the following three physical conditions:

$$\begin{aligned}&\int_{S^{n-1}} f(x, \hat{\theta}, \hat{\omega}) \, \mathrm{d}s(\hat{\theta}) = \int_{S^{n-1}} f(x, \hat{\theta}, \hat{\omega}) \, \mathrm{d}s(\hat{\omega}) = 1,\\ &f(x, \hat{\theta}, \hat{\omega}) \geqslant 0, \qquad x \in \mathbb{R}^n, \quad \hat{\theta}, \hat{\omega} \in S^{n-1},\\ &f(x, \hat{\theta}, \hat{\omega}) = f(x, -\hat{\omega}, -\hat{\theta}), \qquad \hat{\theta}, \hat{\omega} \in S^{n-1}.\end{aligned} \tag{2.2}$$

The energy fluency and the energy current density corresponding to given radiance are defined by

$$\varphi(x,t) = \int_{S^{n-1}} I(x,t,\hat{\theta})\,\mathrm{d}s(\hat{\theta}), \qquad \vec{J}(x,t) = \int_{S^{n-1}} I(x,t,\hat{\theta})\hat{\theta}\,\mathrm{d}s(\hat{\theta}),$$

respectively. Note that $\varphi(x,t)$ and $\vec{J}(x,t)$ may be considered to be the coefficients of the zeroth- and first-order terms for the linearization of $I(x,t,\hat{\theta})$ with respect to $\hat{\theta}$. For more transport theory the reader should consult, for example, [5].

2.2. *Strong scattering*

Being an integrodifferential equation, the radiative transfer equation, as discussed above, leads easily to numerical problems of prohibitive size if no simplifications are made. The commonly used simplification is called the diffusion approximation, which has been shown to be justified for materials that are much more scattering than absorbing [1].

Let $P : L^2(S^{n-1}) \to \mathrm{span}\{1, \theta_1, \ldots, \theta_n\}$ be an orthogonal projection, which linearizes the dependence on the scattering direction. Denoting the integrodifferential operator induced by the left-hand side of (2.1) by $\mathcal{B}$, we define the diffusion approximation of the radiative transfer equation as

$$P\mathcal{B}PI = 0, \tag{2.3}$$

where I denotes the radiance. Due to the way that the projection P is defined, one should be able to write the diffusion approximation using only the energy fluency φ and the energy current density $\vec{J}$ defined at the end of the previous subsection. Indeed, by a straightforward calculation [8, 2], one sees that equation (2.3) is equivalent to the coupled system

$$\frac{1}{c}\varphi_t = -\nabla\cdot\vec{J} - \mu\varphi, \tag{2.4}$$

$$\frac{1}{c}\vec{J}_t = -\frac{1}{n}\nabla\varphi - (\mu + (I - B)\mu_s)\vec{J}, \tag{2.5}$$

where $I \in \mathbb{R}^{n\times n}$ is the identity matrix and the symmetric matrix $B \in \mathbb{R}^{n\times n}$ is defined by

$$B_{jk} = \frac{n}{|S^{n-1}|}\int_{S^{n-1}}\int_{S^{n-1}} \theta_j\omega_k f(x,\hat{\theta},\hat{\omega})\,\mathrm{d}s(\hat{\theta})\,\mathrm{d}s(\hat{\omega}).$$

In order to handle the boundary conditions corresponding to the diffusion approximation, we need to write the total flux inwards (−) and outwards (+) on the boundary $\partial\Omega$ when the dependence on the scattering direction is linearized. In [8], the linearized radiance is projected on the unit normal at $x \in \partial\Omega$ obtaining the fluxes

$$\Phi_\pm(x,t) = \gamma\varphi(x,t) \pm \tfrac{1}{2}\nu(x)\cdot\vec{J}(x,t), \tag{2.6}$$

where $\nu(x)$ is the outer unit normal of $\partial\Omega$, in two dimensions $\gamma = \frac{1}{\pi}$ and in three dimensions $\gamma = \frac{1}{4}$. Note that the expression for the fluxes $\Phi_\pm$ in (2.6) differs somewhat from the one given in most references. However, since (2.6) is carefully conducted from the mathematical model described above [8] and it also represents natural symmetry between the two fluxes, it is one reasonable choice. Furthermore, note that the sign of the inward flux Φ_- in (2.6) is different from that given in [8, 9]: In this work, the net flux through $\partial\Omega$ is obtained by taking the difference $\Phi_+ - \Phi_-$, i.e. here both the inward and outward fluxes are treated as positive quantities.

3. Forward problem

In this section, we will introduce the forward problem corresponding to the diffusion approximation of the radiative transfer equation assuming that the measurements are static in time. Let $\Omega \subset \mathbb{R}^n$, $n = 2$ or $n = 3$ be a bounded body with a smooth boundary and connected complement and suppose that a time invariant flux Φ is conducted through $\partial\Omega$. Setting the time derivatives to zero in (2.4) and (2.5), solving (2.5) for $\vec{J}$ and substituting into (2.4) and (2.6) we end with the following elliptic boundary value problem for φ:

$$\nabla \cdot K\nabla\varphi - \mu\varphi = 0 \quad \text{in } \Omega, \qquad \gamma\varphi + \tfrac{1}{2}\nu \cdot K\nabla\varphi = \Phi \quad \text{on } \partial\Omega, \tag{3.1}$$

where $\nu = \nu(x)$ is the unit normal pointing out of Ω and

$$K = \frac{1}{n}(\mu + (I - B)\mu_s)^{-1},$$

is symmetric. We claim that under the physically reasonable conditions

$$0 < c_a < \mu < C_a \qquad \text{and} \qquad 0 < \mu_s < C_s, \tag{3.2}$$

problem (3.1) has a unique solution.

Theorem 3.1. *Assume that the absorption and scattering coefficients satisfy (3.2) and equations (2.2) are valid. Then for $\Phi \in H^{-1/2}(\partial\Omega)$, the boundary value problem (3.1) has a unique weak solution $\varphi \in H^1(\Omega)$. Further,*

$$\|\varphi\|_{H^1(\Omega)} \leqslant C\|\Phi\|_{H^{-1/2}(\partial\Omega)}. \tag{3.3}$$

Proof. First of all, by using the conditions on μ, μ_s and the scattering phase function, one easily sees that the matrix K is well defined and positive definite. The claim then follows by using the Lax–Milgram lemma [14] on the variational formulation of (3.1). For further details we refer to [9], where similar analysis is conducted for square integrable input flux. □

In the rest of this work we will forget the scattering coefficient μ_s, which does not appear explicitly in (3.1), and treat the diffusion tensor K and the absorption coefficient μ as the two independent optical parameters. Hence, it is important to note that the result of theorem 3.1 remains valid if we assume that μ satisfies the first part of (3.2) and $K \in \mathbb{R}^{n\times n}$ satisfies

$$c_K I < K < C_K I, \qquad c_K, C_K > 0, \tag{3.4}$$

where the inequalities should be understood in the sense of positive definiteness (similar notation will be used throughout this text). In the rest of this work, we will take equations (3.2) and (3.4), as well as the symmetry of K, for granted.

3.1. Robin-to-Robin boundary map

We assume that our measurement setting is such that we can control the input flux penetrating the object boundary and the flux coming out of the object can be measured. In other words, it is assumed that the data that we can collect using non-invasive methods is the linear Robin-to-Robin boundary map defined by

$$\Upsilon : H^{-1/2}(\partial\Omega) \to H^{-1/2}(\partial\Omega), \qquad \Phi \mapsto \left(\gamma\varphi - \tfrac{1}{2}\nu \cdot K\nabla\varphi\right)\big|_{\partial\Omega},$$

where $\varphi \in H^1(\Omega)$ is the unique weak solution of (3.1) corresponding to the input Φ. To collect all Robin–Robin boundary value pairs is in a pure mathematical sense equivalent to collecting all Neumann–Dirichlet pairs. However, since in real life Robin boundary values are those that can be controlled and measured, they are more easily sampled, and so from the practical point of view the above described Robin-to-Robin operator is the boundary map that should be explored when implementing the factorization method.

The following lemma lists some basic properties of Υ. In what follows, we will denote by $\langle u, v\rangle_{L^2(\partial\Omega)} = \int_{\partial\Omega} uv\, \mathrm{d}S$ the dual pairing between $H^{-1/2}(\partial\Omega)$ and $H^{1/2}(\partial\Omega)$ as well as the $L^2(\partial\Omega)$ inner product.

Lemma 3.2. *The operator $\Upsilon : H^{-1/2}(\partial\Omega) \to H^{-1/2}(\partial\Omega)$ can be written as $T - I$, where $T : H^{-1/2}(\partial\Omega) \to H^{1/2}(\partial\Omega)$ is bounded; in particular, Υ is a Fredholm operator of index 0. Further, $\Upsilon|_{L^2(\partial\Omega)} : L^2(\partial\Omega) \to L^2(\partial\Omega)$ is self-adjoint.*

Proof. First of all, we may clearly write $\Upsilon = T - I$, where

$$T : H^{-1/2}(\partial\Omega) \to H^{1/2}(\partial\Omega) \subset H^{-1/2}(\partial\Omega), \qquad \Phi \mapsto 2\gamma\varphi|_{\partial\Omega},$$

is bounded due to the continuity of the solution map $\Phi \mapsto \varphi$ from $H^{-1/2}(\partial\Omega)$ to $H^1(\Omega)$, given by (3.3), and the trace theorem. Since the embedding $H^{1/2}(\partial\Omega) \hookrightarrow H^{-1/2}(\partial\Omega)$ is compact [13], $T : H^{-1/2}(\partial\Omega) \to H^{-1/2}(\partial\Omega)$ is compact, and it follows that Υ is a Fredholm operator of index 0.

Using the above-derived expansion for Υ, it is easy to see that $\Upsilon|_{L^2(\partial\Omega)} \in \mathcal{L}(L^2(\partial\Omega))$. Let $\Phi_1, \Phi_2 \in L^2(\partial\Omega)$ be two input fluxes and $\varphi_1, \varphi_2 \in H^1(\Omega)$ the corresponding solutions of (3.1). By using Green's formula, (3.1) and the symmetry of K we see that

$$\int_{\partial\Omega} \nu \cdot K\nabla\varphi_2\varphi_1\, \mathrm{d}S = \int_{\partial\Omega} \nu \cdot K\nabla\varphi_1\varphi_2\, \mathrm{d}S.$$

Hence,

$$\langle\Upsilon\Phi_1, \Phi_2\rangle_{L^2(\partial\Omega)} = \gamma^2 \int_{\partial\Omega} \varphi_1\varphi_2\, \mathrm{d}S - \frac{1}{4}\int_{\partial\Omega} (\nu \cdot K\nabla\varphi_1)(\nu \cdot K\nabla\varphi_2)\, \mathrm{d}S = \langle\Phi_1, \Upsilon\Phi_2\rangle_{L^2(\partial\Omega)},$$

which proves that $\Upsilon|_{L^2(\partial\Omega)} : L^2(\partial\Omega) \to L^2(\partial\Omega)$ is self-adjoint. This completes the proof. □

Corollary 3.3. *Let Υ and $\tilde{\Upsilon}$ be the Robin-to-Robin boundary maps corresponding to the pairs (K, μ) and $(\tilde{K}, \tilde{\mu})$, respectively. Then $\Upsilon - \tilde{\Upsilon} \in \mathcal{L}(H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega))$ is self-adjoint. Further, if $K \leqslant \tilde{K}$ and $\mu \leqslant \tilde{\mu}$, with one of the inequalities being strict on a set of non-zero measure, then $\Upsilon - \tilde{\Upsilon}$ is injective.*

Proof. The fact that $\Upsilon - \tilde{\Upsilon}$ maps $H^{-1/2}(\partial\Omega)$ continuously to $H^{1/2}(\partial\Omega)$ is a straightforward consequence of the decomposition of lemma 3.2, and the self-adjointness of $\Upsilon - \tilde{\Upsilon} : H^{-1/2}(\partial\Omega) \to H^{1/2}(\partial\Omega)$ follows from the self-adjointness of the restricted operator $(\Upsilon - \tilde{\Upsilon})|_{L^2(\partial\Omega)} : L^2(\partial\Omega) \to L^2(\partial\Omega)$ through a density argument.

To prove the second part of the claim, let $K \leqslant \tilde{K}$ and $\mu \leqslant \tilde{\mu}$ with one of the inequalities being strict on a set of non-zero measure. Assume that $\Phi \in H^{-1/2}(\partial\Omega)$ satisfies $(\Upsilon - \tilde{\Upsilon})\Phi = 0$ and let $\varphi, \tilde{\varphi} \in H^1(\Omega)$ be the corresponding solutions of (3.1). Clearly,

$$(\varphi - \tilde{\varphi})|_{\partial\Omega} = (\nu \cdot K\nabla\varphi - \nu \cdot \tilde{K}\nabla\tilde{\varphi})|_{\partial\Omega} = 0.$$

On the other hand, denoting $f = (\nu \cdot K\nabla\varphi)|_{\partial\Omega} = (\nu \cdot \tilde{K}\nabla\tilde{\varphi})|_{\partial\Omega}$ and using the minimization properties of φ and $\tilde{\varphi}$, one sees that (cf, for example, [4] and [6])

$$\langle f, \varphi - \tilde{\varphi}\rangle_{L^2(\partial\Omega)} \geqslant 0,$$

where the equality holds if and only if $f = 0$. In consequence, it follows from the unique solvability of (3.1) with Robin data replaced by Neumann data [13] that $\varphi = \tilde{\varphi} = 0$ everywhere in Ω. In particular, $\Phi = \left(\gamma\varphi + \frac{1}{2}\nu \cdot K\nabla\varphi\right)\big|_{\partial\Omega} = 0$, which proves the claim. □

4. Factorization

We will first consider the factorization method with only one inclusion; the generalization for the case of multiple inclusions will be addressed briefly at the end of this work. Let the diffusion matrix K and the absorption coefficient μ be of the form

$$K = \begin{cases} K_0 + \kappa & \text{in } D, \\ K_0 & \text{in } \Omega\backslash\overline{D}, \end{cases} \qquad \mu = \begin{cases} \mu_0 + \delta & \text{in } D, \\ \mu_0 & \text{in } \Omega\backslash\overline{D}, \end{cases} \tag{4.1}$$

where $K_0, \mu_0 \in C^\infty(\Omega)$ are the known background diffusion tensor and absorption coefficient, respectively, D is an open connected subset of Ω with connected complement and a smooth boundary $\partial D \cap \partial\Omega = \emptyset$ and $\kappa, \delta \in C^\infty(\overline{D})$ are the perturbations corresponding to D. In what follows, we will denote the Robin-to-Robin boundary map corresponding to (K, μ) by Υ and the map corresponding to (K_0, μ_0) by Υ_0. Our goal in this section is to prove the following theorem:

Theorem 4.1. *The difference of the boundary maps* $\Upsilon, \Upsilon_0 : H^{-1/2}(\partial\Omega) \to H^{-1/2}(\partial\Omega)$ *can be factorized as* $\Upsilon - \Upsilon_0 = LFL'$, *where* $L : H^{-1/2}(\partial D) \to H^{1/2}(\partial\Omega)$, *its adjoint* $L' : H^{-1/2}(\partial\Omega) \to H^{1/2}(\partial D)$ *and* $F : H^{1/2}(\partial D) \to H^{-1/2}(\partial D)$ *are bounded. In addition,* F *is self-adjoint.*

In the following considerations, as well as in the rest of this paper, on the inner boundary ∂D the unit normal $\nu = \nu(x)$ points out of $\Omega\backslash\overline{D}$ into D—note that this convention differs from that used in, e.g., [4] and [10]. We begin defining L and L' by introducing the following Robin boundary value problem:

$$\begin{aligned} \nabla \cdot K_0 \nabla v - \mu_0 v &= 0 && \text{in } \Omega\backslash\overline{D}, \\ \gamma v + \tfrac{1}{2}\nu \cdot K_0 \nabla v &= 0 && \text{on } \partial\Omega, \\ \gamma v + \tfrac{1}{2}\nu \cdot K_0 \nabla v &= \Psi && \text{on } \partial D, \end{aligned} \tag{4.2}$$

which has a unique solution $v \in H^1(\Omega\backslash\overline{D})$ for $\Psi \in H^{-1/2}(\partial D)$ due to a slight modification of theorem 3.1. Thus, we may define L by

$$L : H^{-1/2}(\partial D) \to H^{1/2}(\partial\Omega), \qquad \Psi \mapsto \left(\gamma v - \tfrac{1}{2}\nu \cdot K_0 \nabla v\right)\big|_{\partial\Omega}.$$

Due to the trace theorem and the continuous dependence on boundary data (3.3), we have

$$\left\|\gamma v - \tfrac{1}{2}\nu \cdot K_0 \nabla v\right\|_{H^{1/2}(\partial\Omega)} = \|2\gamma v\|_{H^{1/2}(\partial\Omega)} \leqslant C\|v\|_{H^1(\Omega\backslash\overline{D})} \leqslant C\|\Psi\|_{H^{-1/2}(\partial D)},$$

and so L is bounded. The adjoint operator L' is given by

$$L' : H^{-1/2}(\partial\Omega) \to H^{1/2}(\partial D), \qquad \Psi' \mapsto \left(\gamma v' - \tfrac{1}{2}\nu \cdot K_0 \nabla v'\right)\big|_{\partial D},$$

where $v' \in H^1(\Omega\backslash\overline{D})$ is the unique solution of

$$\begin{aligned} \nabla \cdot K_0 \nabla v' - \mu_0 v' &= 0 && \text{in } \Omega\backslash\overline{D}, \\ \gamma v' + \tfrac{1}{2}\nu \cdot K_0 \nabla v' &= \Psi' && \text{on } \partial\Omega, \\ \gamma v' + \tfrac{1}{2}\nu \cdot K_0 \nabla v' &= 0 && \text{on } \partial D. \end{aligned}$$

Indeed, with the help of the boundary conditions that v and v' satisfy, we may write

$$\begin{aligned} \langle \Psi', L\Psi \rangle_{L^2(\partial\Omega)} &= \int_{\partial\Omega} \left(\gamma v' + \frac{1}{2}\nu \cdot K_0 \nabla v'\right)\left(\gamma v - \frac{1}{2}\nu \cdot K_0 \nabla v\right) \mathrm{d}S \\ &= \gamma \int_{\partial\Omega} \nu \cdot K_0 \nabla v' v \, \mathrm{d}S - \gamma \int_{\partial\Omega} \nu \cdot K_0 \nabla v v' \, \mathrm{d}S \end{aligned}$$

$$= \gamma \int_{\partial D} \nu \cdot K_0 \nabla v v' \, \mathrm{d}S - \gamma \int_{\partial D} \nu \cdot K_0 \nabla v' v \, \mathrm{d}S$$
$$= \int_{\partial D} \left(\gamma v + \frac{1}{2} \nu \cdot K_0 \nabla v \right) \left(\gamma v' - \frac{1}{2} \nu \cdot K_0 \nabla v' \right) \mathrm{d}S$$
$$= \langle \Psi, L' \Psi' \rangle_{L^2(\partial D)},$$

where we also used Green's formula and the symmetry of K_0. As an adjoint of a linear bounded operator, L' is linear and bounded.

Before we can introduce the third operator needed for the factorization of theorem 4.1, we need to consider some notational details. On the inner boundary ∂D we define

$$v^{\pm}(x) = \lim_{t \to 0^+} v(x \pm t\nu), \qquad (\nu \cdot K \nabla v)^{\pm}(x) = \lim_{t \to 0^+} \nu \cdot (K \nabla v)(x \pm t\nu),$$

for $x \in \partial D$ with $\nu(x)$ the unit normal pointing into D, and further

$$[v]_{\partial D} = v^+ - v^- \qquad \text{and} \qquad [\nu \cdot K \nabla v]_{\partial D} = (\nu \cdot K \nabla v)^+ - (\nu \cdot K \nabla v)^-.$$

Note that the signs of the above-defined limits are the opposite compared to the definitions given in [4] because ν points here in the opposite direction.

The inner boundary operator $F : H^{1/2}(\partial D) \to H^{-1/2}(\partial D)$ is defined through $F = F_\kappa - F_0$, where

$$F_\kappa : \Theta \mapsto \left(\gamma w + \tfrac{1}{2} \nu \cdot K \nabla w \right)^- \big|_{\partial D}, \qquad F_0 : \Theta \mapsto \left(\gamma w_0 + \tfrac{1}{2} \nu \cdot K_0 \nabla w_0 \right)^- \big|_{\partial D},$$

and $w, w_0 \in H^1(\Omega \backslash \partial D)$ are the unique weak solutions of the diffraction problem

$$\begin{aligned} &\nabla \cdot K \nabla w - \mu w = 0 && \text{in } \Omega \backslash \partial D, \\ &\gamma w + \tfrac{1}{2} \nu \cdot K \nabla w = 0 && \text{on } \partial \Omega, \\ &2\gamma [w]_{\partial D} = -[\nu \cdot K \nabla w]_{\partial D} = \Theta, \end{aligned} \tag{4.3}$$

corresponding to the pairs (K, μ), given by (4.1), and (K_0, μ_0), respectively. Note that the conditions on the inner boundary in (4.3) are equivalent to the following: the flux going into the region D jumps by Θ on ∂D and the flux coming out of D is continuous over ∂D.

Lemma 4.2. *The operator $F : H^{1/2}(\partial D) \to H^{-1/2}(\partial D)$ is well defined, bounded and self-adjoint.*

Proof. The fact that (4.3) is uniquely solvable and the solution depends continuously on the data follows from material in [12], and so the continuity of $F : H^{1/2}(\partial D) \to H^{-1/2}(\partial D)$ is a consequence of the trace theorem and the boundedness of the map

$$H(\mathrm{div}, \Omega \backslash \overline{D}) \to H^{-1/2}(\partial D), \qquad \mathbf{v} \mapsto (\nu \cdot \mathbf{v})^- |_{\partial D}, \tag{4.4}$$

where $H(\mathrm{div}, \Omega \backslash \overline{D}) = \{\mathbf{v} \in (L^2(\Omega \backslash \overline{D}))^n \mid \nabla \cdot \mathbf{v} \in L^2(\Omega \backslash \overline{D})\}$, cf, e.g., [6].

Let us next consider the self-adjointness. For $\Theta_1, \Theta_2 \in H^{1/2}(\partial D)$ let $w_1, w_2 \in H^1(\Omega \backslash \partial D)$ be the corresponding solutions of the diffraction problem (4.3) with the pair (K, μ). By using the boundary conditions that w_2 satisfies, we may write

$$\begin{aligned} \langle F_\kappa \Theta_1, \Theta_2 \rangle_{L^2(\partial D)} &= \gamma \int_{\partial D} w_1^- ((\nu \cdot K \nabla w_2)^- - (\nu \cdot K \nabla w_2)^+) \, \mathrm{d}S \\ &\quad + \gamma \int_{\partial D} (\nu \cdot K \nabla w_1)^- \left(w_2^+ - w_2^- \right) \mathrm{d}S \\ &= \gamma \left\{ \int_{\partial D} (\nu \cdot K \nabla w_2)^- w_1^- \, \mathrm{d}S - \int_{\partial D} (\nu \cdot K \nabla w_1)^- w_2^- \, \mathrm{d}S \right\} \\ &\quad + \gamma \left\{ \int_{\partial D} (\nu \cdot K \nabla w_1)^- w_2^+ \, \mathrm{d}S - \int_{\partial D} (\nu \cdot K \nabla w_2)^+ w_1^- \, \mathrm{d}S \right\}. \end{aligned} \tag{4.5}$$

Due to Green's formula, the term on the second to last row of (4.5) equals

$$\gamma\left\{\int_{\partial\Omega}\nu\cdot K\nabla w_1 w_2\,\mathrm{d}S-\int_{\partial\Omega}\nu\cdot K\nabla w_2 w_1\,\mathrm{d}S\right\}=0,$$

where we used the boundary conditions on the outer boundary $\partial\Omega$. Hence, by using Green's formula and the boundary conditions of (4.3) on ∂D, we obtain

$$\begin{aligned}\langle F_\kappa\Theta_1,\Theta_2\rangle_{L^2(\partial D)}&=\int_{\partial D}((\nu\cdot K\nabla w_1)^++\Theta_1)\gamma w_2^+\,\mathrm{d}S-\int_{\partial D}\frac{1}{2}(\nu\cdot K\nabla w_2)^+\big(2\gamma w_1^+-\Theta_1\big)\,\mathrm{d}S\\&=\int_{\partial D}\left(\gamma w_2+\frac{1}{2}\nu\cdot K\nabla w_2\right)^+\Theta_1\,\mathrm{d}S\\&=\int_{\partial D}\left(\gamma w_2+\frac{1}{2}\nu\cdot K\nabla w_2\right)^-\Theta_1\,\mathrm{d}S\\&=\langle F_\kappa\Theta_2,\Theta_1\rangle_{L^2(\partial D)}.\end{aligned}$$

Since a similar reasoning also holds for F_0, we have altogether shown that F is self-adjoint. □

Now it is time to provide a proof for theorem 4.1.

Proof of theorem 4.1. For a fixed input flux $\Phi\in H^{-1/2}(\partial\Omega)$, denote by $\varphi,\varphi_0\in H^1(\Omega)$ the solutions of the forward problem (3.1) corresponding to the pairs (K,μ) and (K_0,μ_0), respectively. Clearly, $(\varphi-\varphi_0)|_{\Omega\setminus\overline{D}}$ solves (4.2) for $\Psi=\big\{\gamma(\varphi-\varphi_0)+\frac{1}{2}\nu\cdot K_0\nabla(\varphi-\varphi_0)\big\}^-\big|_{\partial D}$ and, in particular,

$$\begin{aligned}L\big(\big\{\gamma(\varphi-\varphi_0)+\tfrac{1}{2}\nu\cdot K_0\nabla(\varphi-\varphi_0)\big\}^-\big|_{\partial D}\big)&=\big\{\gamma(\varphi-\varphi_0)-\tfrac{1}{2}\nu\cdot K_0\nabla(\varphi-\varphi_0)\big\}\big|_{\partial\Omega}\\&=(\Upsilon-\Upsilon_0)\Phi.\end{aligned}$$

By introducing the operator $G_\kappa:\Phi\mapsto\big(\gamma\varphi+\frac{1}{2}\nu\cdot K\nabla\varphi\big)^-\big|_{\partial D}=\big(\gamma\varphi+\frac{1}{2}\nu\cdot K_0\nabla\varphi\big)^-\big|_{\partial D}$ and setting $G=G_\kappa-G_0$, where G_0 is the counterpart of G_κ corresponding to φ_0, we have so far derived the factorization

$$\Upsilon-\Upsilon_0=LG. \tag{4.6}$$

Note that G is a well-defined bounded operator from $H^{-1/2}(\partial\Omega)$ to $H^{-1/2}(\partial D)$ due to (3.3), the trace theorem and (4.4).

The next task is to calculate the dual operator $G_\kappa':H^{1/2}(\partial D)\to H^{1/2}(\partial\Omega)$ of G_κ. To this end, consider $w\in H^1(\Omega\setminus\partial D)$ the solution of diffraction problem (4.3) corresponding to $\Theta\in H^{1/2}(\partial D)$ and (K,μ). With the help of the jump conditions $[\varphi]_{\partial D}=[\nu\cdot K\nabla\varphi]_{\partial D}=0$ (cf [12]), the Green's formula in both interior and exterior regions, and the boundary conditions on φ and w, we deduce

$$\begin{aligned}\langle G_\kappa\Phi,\Theta\rangle_{L^2(\partial D)}&=\int_{\partial D}\left(\gamma\varphi+\frac{1}{2}\nu\cdot K\nabla\varphi\right)^-\Theta\,\mathrm{d}S\\&=\gamma\int_{\partial D}\nu\cdot K\nabla\varphi(w^+-w^-)\,\mathrm{d}S-\gamma\int_{\partial D}((\nu\cdot K\nabla w)^+-(\nu\cdot K\nabla w)^-)\varphi\,\mathrm{d}S\\&=\gamma\int_{\partial D}(\nu\cdot K\nabla w)^-\varphi\,\mathrm{d}S-\gamma\int_{\partial D}\nu\cdot K\nabla\varphi w^-\,\mathrm{d}S\\&=\gamma\int_{\partial\Omega}\nu\cdot K\nabla\varphi w\,\mathrm{d}S-\gamma\int_{\partial\Omega}\nu\cdot K\nabla w\varphi\,\mathrm{d}S\\&=\int_{\partial\Omega}\frac{1}{2}\nu\cdot K\nabla\varphi\left(\gamma w-\frac{1}{2}\nu\cdot K\nabla w\right)\mathrm{d}S+\int_{\partial\Omega}\left(\gamma w-\frac{1}{2}\nu\cdot K\nabla w\right)\gamma\varphi\,\mathrm{d}S\\&=\left\langle\Phi,\gamma w-\frac{1}{2}\nu\cdot K\nabla w\right\rangle_{L^2(\partial\Omega)},\end{aligned}$$

which shows that $G'_\kappa\Theta = \big(\gamma w - \frac{1}{2}\nu\cdot K\nabla w\big)\big|_{\partial\Omega} = \big(\gamma w - \frac{1}{2}\nu\cdot K_0\nabla w\big)\big|_{\partial\Omega} \in H^{1/2}(\partial\Omega)$ due to the trace theorem and the outer boundary condition of (4.3). Hence, with $w_0 \in H^1(\Omega\backslash\partial D)$ being the solution of (4.3) corresponding to Θ and (K_0, μ_0), we have

$$G'\Theta = \big\{\gamma(w - w_0) - \tfrac{1}{2}\nu\cdot K_0\nabla(w - w_0)\big\}\big|_{\partial\Omega}.$$

The restriction $(w - w_0)|_{\Omega\backslash\overline{D}}$ solves (4.2) for $\Psi = \big\{\gamma(w-w_0)+\frac{1}{2}\nu\cdot K_0\nabla(w-w_0)\big\}^-\big|_{\partial D}$, which means that

$$L\big(\big\{\gamma(w - w_0) + \tfrac{1}{2}\nu\cdot K_0\nabla(w - w_0)\big\}^-\big|_{\partial D}\big) = \big\{\gamma(w - w_0) - \tfrac{1}{2}\nu\cdot K_0\nabla(w - w_0)\big\}\big|_{\partial\Omega},$$

which equals $G'\Theta$. Due to the way $F : H^{1/2}(\partial D) \to H^{-1/2}(\partial D)$ is defined and since $\Theta \in H^{1/2}(\partial D)$ was chosen arbitrarily, the above relation is equivalent to $G' = LF$. Taking the transpose of this and plugging it into (4.6), we obtain

$$\Upsilon - \Upsilon_0 = LF'L' = LFL',$$

which is what we set out to prove. □

5. Further properties of *F*

To use the factorization given in theorem 4.1 for inclusion characterization in the same way as in [4], one needs to show that $F : H^{1/2}(\partial D) \to H^{-1/2}(\partial D)$ is self-adjoint, bijective and either positive or negative definite. The self-adjointness is a fundamental property of F, but the latter two conditions hold only if suitable conditions are imposed on the perturbations κ and δ.

Physically speaking, the inner boundary operator F is positive if and only if the existence of the inclusion $D \subset \Omega$ decreases the amount of absorbed photons inside the body Ω for any input flux. In the framework of the diffusion approximation, a sufficient condition is

$$\kappa \leqslant 0 \qquad \text{and} \qquad \delta \leqslant 0 \quad \text{in } D, \tag{5.1}$$

where the first inequality is to be interpreted in the sense of positive definiteness and one of the inequalities is strict on a set of non-zero measure in D. Similarly, F is negative definite if

$$\kappa \geqslant 0 \qquad \text{and} \qquad \delta \geqslant 0 \quad \text{in } D, \tag{5.2}$$

with one of the inequalities being strict on a set of non-zero measure.

Lemma 5.1. *If condition (5.1) is valid, then $F : H^{1/2}(\partial D) \to H^{-1/2}(\partial D)$ is positive definite. On the other hand, if (5.2) holds, F is negative definite. In either of these cases F is injective.*

Proof. We start by showing that the solution of (4.3), $w \in H^1(\Omega\backslash\partial D)$, corresponding to $\Theta \in H^{1/2}(\partial D)$ and the pair (K, μ), is the unique minimizer of the quadratic functional $E_\kappa(\cdot,\cdot)$, defined by

$$E_\kappa(u, v) = \int_\Omega K\nabla u\cdot\nabla v\,\mathrm{d}x + \int_\Omega \mu uv\,\mathrm{d}x + 2\gamma\int_{\partial\Omega} uv\,\mathrm{d}S + 2\gamma\int_{\partial D}(u^-v^- - u^+v^+)\,\mathrm{d}S, \tag{5.3}$$

over the subset

$$H_\Theta = \{\tilde{w} \in H^1(\Omega\backslash\partial D) \mid 2\gamma[\tilde{w}]_{\partial D} = \Theta\}.$$

Indeed, denoting $v = \tilde{w} - w$ for an arbitrary $\tilde{w} \in H_\Theta$, we have

$$E_\kappa(\tilde{w}, \tilde{w}) = E_\kappa(w, w) + E_\kappa(v, v) + 2E_\kappa(w, v). \tag{5.4}$$

By using Green's formula, the boundary conditions of (4.3) and noting that $[v]_{\partial D} = 0$, we may write

$$\int_\Omega K\nabla w \cdot \nabla v \,\mathrm{d}x = \int_{\partial D} ((\nu \cdot K\nabla w)^- - (\nu \cdot K\nabla w)^+) v \,\mathrm{d}S - \int_\Omega \mu w v \,\mathrm{d}x + \int_{\partial\Omega} \nu \cdot K\nabla w v \,\mathrm{d}S$$
$$= \int_{\partial D} \Theta v \,\mathrm{d}S - \int_\Omega \mu w v \,\mathrm{d}x - 2\gamma \int_{\partial\Omega} w v \,\mathrm{d}S,$$

from which it follows that

$$E_\kappa(w, v) = \int_{\partial D} \Theta v \,\mathrm{d}S + 2\gamma \int_{\partial D} (w^- - w^+) v \,\mathrm{d}S = 0.$$

Moreover, since $[v]_{\partial D} = 0$, the inner boundary term of $E_\kappa(v, v)$ vanishes, meaning that $E_\kappa(v, v) \geqslant 0$ with the equality holding if and only if $v = 0$. Combining the material above, we have altogether established that $E_\kappa(w, w) \leqslant E_\kappa(\tilde{w}, \tilde{w})$, where the equality holds if and only if $\tilde{w} = w$. In the same way one also sees that the solution of (4.3) corresponding to $\Theta \in H^{1/2}(\partial D)$ and (K_0, μ_0) is the unique minimizer of the quadratic form $E_0(\cdot, \cdot)$, obtained by replacing (K, μ) with (K_0, μ_0) in (5.3), over the very same set H_Θ.

On the other hand, for $\Theta \in H^{1/2}(\partial D)$ and w, defined as above, it also holds that

$$\begin{aligned}\langle F_\kappa \Theta, \Theta\rangle_{L^2(\partial D)} &= \int_{\partial D} \left(\gamma w + \frac{1}{2}\nu \cdot K\nabla w\right)^- \Theta \,\mathrm{d}S \\ &= \int_{\partial D} \frac{1}{2}(\nu \cdot K\nabla w)^- \Theta \,\mathrm{d}S - \int_{\partial D} \gamma w^+ \Theta \,\mathrm{d}S + \gamma \int_{\partial D} (w^- + w^+)\Theta \,\mathrm{d}S \\ &= -\gamma \left\{ \int_{\partial D} (\nu \cdot K\nabla w)^- w^- \,\mathrm{d}S - \int_{\partial D} (\nu \cdot K\nabla w)^+ w^+ \,\mathrm{d}S \right. \\ &\quad \left. + 2\gamma \int_{\partial D} ((w^-)^2 - (w^+)^2) \,\mathrm{d}S \right\},\end{aligned}$$

where the last equality follows by writing Θ in two ways: using the normal derivatives in the second term and the Dirichlet boundary values in the first and third terms. With the help of Green's formula, in both inner and outer regions, and the boundary condition that w satisfies on $\partial\Omega$, one sees that

$$\langle F_\kappa \Theta, \Theta\rangle_{L^2(\partial D)} = -\gamma E_\kappa(w, w). \tag{5.5}$$

Denoting the solution of (4.3) corresponding to Θ and the pair (K_0, μ_0) by $w_0 \in H^1(\Omega\backslash\partial D)$, we obtain in similar fashion that

$$\langle F_0 \Theta, \Theta\rangle_{L^2(\partial D)} = -\gamma E_0(w_0, w_0). \tag{5.6}$$

Due to the minimization properties of w and w_0 considered above, for $\kappa \leqslant 0$ and $\delta \leqslant 0$, with one of the inequalities being strict on a set of non-zero measure, we have

$$E_\kappa(w, w) < E_\kappa(w_0, w_0) \leqslant E_0(w_0, w_0).$$

Similarly, for $\kappa \geqslant 0$ and $\delta \geqslant 0$, with one of the inequalities being strict on a set of non-zero measure, it holds that

$$E_0(w_0, w_0) < E_0(w, w) \leqslant E_\kappa(w, w).$$

Now the claim follows from these estimates together with (5.5) and (5.6). □

We still need to say something about the surjectivity of F. In order to be successful in this task, we need to define a couple of auxiliary operators. The Robin-to-Robin map corresponding to the pair (K, μ), given in (4.1), and the interior region D is defined by

$$\Upsilon^D : H^{-1/2}(\partial D) \to H^{-1/2}(\partial D), \qquad \Phi_{\mathrm{in}} \mapsto \left(\gamma\phi + \tfrac{1}{2}\nu \cdot K\nabla\phi\right)^+\big|_{\partial D},$$

where $\phi \in H^1(D)$ satisfies the boundary value problem

$$\begin{aligned} &\nabla \cdot K\nabla\phi - \mu\phi = 0 && \text{in } D, \\ &\left(\gamma\phi - \tfrac{1}{2}\nu \cdot K\nabla\phi\right)^+ = \Phi_{\text{in}} && \text{on } \partial D. \end{aligned} \tag{5.7}$$

Note that Υ^D has all the properties given in lemma 3.2; the sign changes in the boundary conditions are due to the fact that the unit normal ν points into the region D not out of it. The Robin-to-Robin map $\Upsilon_0^D : H^{-1/2}(\partial D) \to H^{-1/2}(\partial D)$ corresponding to the background pair (K_0, μ_0) is defined in similar fashion. Further, we introduce the exterior Robin-to-Robin boundary map:

$$\Upsilon^{\Omega\backslash\overline{D}} : H^{-1/2}(\partial D) \to H^{-1/2}(\partial D), \qquad \Phi_{\text{out}} \mapsto \left(\gamma\psi - \tfrac{1}{2}\nu \cdot K_0\nabla\psi\right)^-\big|_{\partial D},$$

where $\psi \in H^1(\Omega\backslash\overline{D})$ is the solution of

$$\begin{aligned} &\nabla \cdot K_0\nabla\psi - \mu_0\psi = 0 && \text{in } \Omega\backslash\overline{D}, \\ &\left(\gamma\psi + \tfrac{1}{2}\nu \cdot K_0\nabla\psi\right)^- = \Phi_{\text{out}} && \text{on } \partial D, \\ &\gamma\psi + \tfrac{1}{2}\nu \cdot K_0\nabla\psi = 0 && \text{on } \partial\Omega. \end{aligned} \tag{5.8}$$

One easily sees that $\Upsilon^{\Omega\backslash\overline{D}}$ also has the properties of lemma 3.2.

The following two technical lemmas give information that is essential when proving the surjectivity of F.

Lemma 5.2. *The operator $I - \Upsilon^D\Upsilon^{\Omega\backslash\overline{D}}$ maps $H^{-1/2}(\partial D)$ injectively to $H^{1/2}(\partial D)$.*

Proof. First of all, let us prove that $\mathcal{R}(I - \Upsilon^D\Upsilon^{\Omega\backslash\overline{D}}) \subset H^{1/2}(\partial D)$. As in the proof of lemma 3.2, one easily sees that $\Upsilon^{\Omega\backslash\overline{D}}$ can be given in the form $T^{\Omega\backslash\overline{D}} - I$, where $T^{\Omega\backslash\overline{D}} : H^{-1/2}(\partial D) \to H^{1/2}(\partial D)$. Using this together with the analogous representation $\Upsilon^D = T^D - I$, where $T^D : H^{-1/2}(\partial D) \to H^{1/2}(\partial D)$, we obtain

$$\Upsilon^D\Upsilon^{\Omega\backslash\overline{D}} = I - T^D - T^{\Omega\backslash\overline{D}} + T^D T^{\Omega\backslash\overline{D}},$$

which proves the claim.

In order to prove the injectivity, assume that $\Upsilon^D\Upsilon^{\Omega\backslash\overline{D}}\Phi_{\text{out}} = \Phi_{\text{out}}$ for some $\Phi_{\text{out}} \in H^{-1/2}(\partial D)$, i.e. $\Phi_{\text{out}} \in \mathcal{N}(I - \Upsilon^D\Upsilon^{\Omega\backslash\overline{D}})$. We define $u \in H^1(\Omega\backslash\overline{D})$ to be the unique solution of (5.8) for this flux Φ_{out}, and continue u to the inner region D as the unique solution of (5.7) with the input $\Phi_{\text{in}} = \Upsilon^{\Omega\backslash\overline{D}}\Phi_{\text{out}} = \left(\gamma u - \frac{1}{2}\nu \cdot K\nabla u\right)^-\big|_{\partial D}$. Combining this with the original assumption on Φ_{out}, we deduce that

$$\left[\gamma u - \tfrac{1}{2}\nu \cdot K\nabla u\right]_{\partial D} = \left[\gamma u + \tfrac{1}{2}\nu \cdot K\nabla u\right]_{\partial D} = 0,$$

or in other words

$$[u]_{\partial D} = [\nu \cdot K\nabla u]_{\partial D} = 0.$$

Since also $\left(\gamma u + \frac{1}{2}\nu \cdot K\nabla u\right)\big|_{\partial\Omega} = 0$ and clearly $u \in H^1(\Omega\backslash\partial D)$, it follows from the unique solvability of (4.3) that $u = 0$. In particular, $\Phi_{\text{out}} = \left(\gamma u + \frac{1}{2}\nu \cdot K\nabla u\right)^-\big|_{\partial D} = 0$, from which it follows that $\mathcal{N}(I - \Upsilon^D\Upsilon^{\Omega\backslash\overline{D}}) = \{0\}$. □

In what follows, we will assume for simplicity that K_0 and κ are scalar functions.

Lemma 5.3. *Let K_0 and κ be scalar functions and assume that either (5.1) holds and κ is negative on ∂D or (5.2) is valid and κ is positive on ∂D. Then the map $\Upsilon^D - \Upsilon_0^D : H^{-1/2}(\partial D) \to H^{1/2}(\partial D)$ is bijective.*

Proof. To begin with, the injectivity of $\Upsilon^D - \Upsilon_0^D$ follows straight away from corollary 3.3. Our plan is to prove that $\Upsilon^D - \Upsilon_0^D : H^{-1/2}(\partial D) \to H^{1/2}(\partial D)$ is a Fredholm operator of index 0, whence the surjectivity follows from the injectivity. By using the decomposition derived in lemma 3.2, for $\Phi_{\text{in}} \in H^{-1/2}(\partial D)$ we may write

$$\left(\Upsilon^D - \Upsilon_0^D\right)\Phi_{\text{in}} = 2\gamma(\phi - \phi_0)^+|_{\partial D},$$

where $\phi, \phi_0 \in H^1(D)$ are the solutions of (5.7) corresponding to the pairs (K, μ) and (K_0, μ_0), respectively. Hence, by defining auxiliary operators $B, T : H^{-1/2}(\partial D) \to H^{1/2}(\partial D)$ through

$$B : \Phi_{\text{in}} \mapsto \left(\left(\frac{K_0}{K} - 1\right)\phi_0\right)^+\Bigg|_{\partial D}, \qquad T : \Phi_{\text{in}} \mapsto \left(\phi - \frac{K_0}{K}\phi_0\right)^+\Bigg|_{\partial D}, \tag{5.9}$$

we have $\Upsilon^D - \Upsilon_0^D = 2\gamma(B + T)$. We claim that B is bijective and T is compact.

Indeed, by assumption $K_0/K - 1$ is smooth and does not equal zero anywhere on ∂D, and so for any $g \in H^{1/2}(\partial D)$ the problem

$$\nabla \cdot K_0 \nabla u - \mu_0 u = 0 \quad \text{in } D, \qquad \left(\frac{K_0}{K} - 1\right) u = g \quad \text{on } \partial D, \tag{5.10}$$

has a unique solution $u \in H^1(D)$ that depends continuously on the data [13]. In consequence, the mapping

$$\tilde{B} : H^{1/2}(\partial D) \to H^{-1/2}(\partial D), \qquad g \mapsto \left(\gamma u - \tfrac{1}{2}\nu \cdot K_0 \nabla u\right)^+\big|_{\partial D},$$

is well defined, and also continuous, by the trace theorem and an obvious variant of (4.4). Using the unique solvability of (5.7) and (5.10), it is easy to see that $\tilde{B}$ is the inverse of B, which proves the first part of the claim.

Let us next consider the non-homogeneous boundary value problem

$$\begin{aligned} &\nabla \cdot K \nabla u - \mu u = f && \text{in } D, \\ &\left(\gamma u - \tfrac{1}{2}\nu \cdot K \nabla u\right)^+ = \Psi && \text{on } \partial D. \end{aligned} \tag{5.11}$$

Due to the regularity theory of elliptic partial differential equations, if $f \in L^2(D)$ and $\Psi \in H^{1/2}(\partial D)$, equation (5.11) has a unique solution $u \in H^2(D)$ and, in addition, the solution map

$$T_1 : L^2(D) \times H^{1/2}(\partial D) \to H^2(D), \qquad (f, \Psi) \mapsto u,$$

is continuous [13].

Let $\phi, \phi_0 \in H^1(D)$ still be the solutions of (5.7) corresponding to the input flux $\Phi_{\text{in}} \in H^{-1/2}(\partial D)$ and the pairs (K, μ) and (K_0, μ_0), respectively. By a straightforward calculation, one sees that the difference $\phi - K_0/K\phi_0$ satisfies equation (5.11) for

$$\begin{aligned} f &= \left(\mu\frac{K_0}{K} - \mu_0\right)\phi_0 - \nabla \cdot \phi_0 K \nabla \frac{K_0}{K}, \\ \Psi &= \left\{\gamma\left(1 - \frac{K_0}{K}\right)\phi_0 + \frac{1}{2}\nu \cdot \phi_0 K \nabla \frac{K_0}{K}\right\}^+\Bigg|_{\partial D}. \end{aligned}$$

Clearly, the operator $T_2 : H^1(D) \to L^2(D) \times H^{1/2}(\partial D)$,

$$v \mapsto \left(\left(\mu\frac{K_0}{K} - \mu_0\right)v - \nabla \cdot vK\nabla\frac{K_0}{K}, \gamma\left(1 - \frac{K_0}{K}\right)v + \frac{1}{2}\nu \cdot vK\nabla\frac{K_0}{K}\right),$$

is well defined and bounded, and so putting the above material together, we have

$$\phi - \frac{K_0}{K}\phi_0 = T_1 T_2 \phi_0 \in H^2(D),$$

where $T_1T_2 : H^1(D) \to H^2(D)$ is bounded. By using this together with the trace theorem and continuous dependence on boundary data in (5.7), we deduce that T, given in (5.9), maps $H^{-1/2}(\partial D)$ continuously to $H^{3/2}(\partial D)$. In consequence, due to the compactness of the imbedding $H^{3/2}(\partial D) \hookrightarrow H^{1/2}(\partial D)$, $T : H^{-1/2}(\partial D) \to H^{1/2}(\partial D)$ is compact.

Hence, $\Upsilon^D - \Upsilon_0^D : H^{-1/2}(\partial D) \to H^{1/2}(\partial D)$ can be given as a sum of an invertible and a compact operator, meaning that it is a Fredholm operator of index 0, and so the bijectivity of $\Upsilon^D - \Upsilon_0^D$ follows from its injectivity. □

Now we have introduced enough weaponry for stating a result about the bijectivity of F.

Lemma 5.4. *Suppose that the assumptions of lemma 5.3 hold. Then the operator $F : H^{1/2}(\partial D) \to H^{-1/2}(\partial D)$ is bijective.*

Proof. The injectivity of $F : H^{1/2}(\partial D) \to H^{-1/2}(\partial D)$ follows from lemma 5.1. Hence, all we have to prove is that F is surjective: Let $\Psi \in H^{-1/2}(\partial D)$ be arbitrary. According to lemmas 5.3 and 5.2, there exists $\Phi_{\text{in}}^0 \in H^{-1/2}(\partial D)$ such that

$$\left(\Upsilon^D - \Upsilon_0^D\right)\Phi_{\text{in}}^0 = (I - \Upsilon^D \Upsilon^{\Omega\setminus\overline{D}})\Psi. \tag{5.12}$$

Let us define $w_0 \in H^1(D)$ as the unique solution of (5.7) with the flux Φ_{in}^0 satisfying (5.12) and (K, μ) replaced with (K_0, μ_0), and continue w_0 to the exterior region $\Omega\setminus\overline{D}$ as the H^1-solution of (5.8) with the flux $\Phi_{\text{out}}^0 = \left(\gamma w_0 + \frac{1}{2}\nu \cdot K_0 \nabla w_0\right)^+\big|_{\partial D}$. Finally, we set $\Theta = 2\gamma[w_0]_{\partial D} \in H^{1/2}(\partial D)$ and claim that $F\Theta = \Psi$.

To begin with, it is easy to see that $w_0 \in H^1(\Omega\setminus\partial D)$ is the solution of (4.3) with (K_0, μ_0) and the input Θ defined above; let $w_\kappa \in H^1(\Omega\setminus\partial D)$ be the solution of (4.3) corresponding to the pair (K, μ) and the same input Θ. To simplify our notation let us define a few auxiliary fluxes:

$$\begin{aligned}
\Phi_{\text{in}}^\kappa &= \left(\gamma w_\kappa - \tfrac{1}{2}\nu \cdot K \nabla w_\kappa\right)^+\big|_{\partial D}, \\
\Phi_{\text{out}}^\kappa &= \left(\gamma w_\kappa + \tfrac{1}{2}\nu \cdot K \nabla w_\kappa\right)^+\big|_{\partial D} = \left(\gamma w_\kappa + \tfrac{1}{2}\nu \cdot K \nabla w_\kappa\right)^-\big|_{\partial D}, \\
\left(\Phi_{\text{in}}^0\right)^- &= \left(\gamma w_0 - \tfrac{1}{2}\nu \cdot K_0 \nabla w_0\right)^-\big|_{\partial D}, \\
\left(\Phi_{\text{in}}^\kappa\right)^- &= \left(\gamma w_\kappa - \tfrac{1}{2}\nu \cdot K \nabla w_\kappa\right)^-\big|_{\partial D}.
\end{aligned}$$

Note that due to the jump conditions of (4.3), Φ_{out}^0 and Φ_{out}^κ are continuous over ∂D whereas $\Phi_{\text{in}}^\kappa - \left(\Phi_{\text{in}}^\kappa\right)^- = \Phi_{\text{in}}^0 - \left(\Phi_{\text{in}}^0\right)^- = \Theta$. With the help of (4.3) and the way Υ^D, Υ_0^D and $\Upsilon^{\Omega\setminus\overline{D}}$ are defined, we may write

$$\begin{aligned}
\Phi_{\text{out}}^\kappa - \Phi_{\text{out}}^0 &= \Upsilon^D \Phi_{\text{in}}^\kappa - \Upsilon_0^D \Phi_{\text{in}}^0 = \Upsilon^D\left(\left(\Phi_{\text{in}}^\kappa\right)^- + \Theta\right) - \Upsilon_0^D \Phi_{\text{in}}^0 \\
&= \left(\Upsilon^D - \Upsilon_0^D\right)\Phi_{\text{in}}^0 + \Upsilon^D\left(\left(\Phi_{\text{in}}^\kappa\right)^- - \left(\Phi_{\text{in}}^0\right)^-\right) \\
&= (I - \Upsilon^D \Upsilon^{\Omega\setminus\overline{D}})\Psi + \Upsilon^D \Upsilon^{\Omega\setminus\overline{D}}\left(\Phi_{\text{out}}^\kappa - \Phi_{\text{out}}^0\right),
\end{aligned}$$

where we also used (5.12). In consequence,

$$(I - \Upsilon^D \Upsilon^{\Omega\setminus\overline{D}})\left(\left(\Phi_{\text{out}}^\kappa - \Phi_{\text{out}}^0\right) - \Psi\right) = 0,$$

from which it follows by lemma 5.2 that, actually,

$$F\Theta = \Phi_{\text{out}}^\kappa - \Phi_{\text{out}}^0 = \Psi.$$

Since $\Psi \in H^{-1/2}(\partial D)$ was chosen arbitrarily, this completes the proof. □

6. Characterizing the inclusion

From now on we will assume that the conditions of lemma 5.3 hold, i.e. K_0 and κ are scalars, and either (5.1) holds and κ is negative on ∂D or (5.2) holds and κ is positive on ∂D. According to lemmas 4.2, 5.4 and 5.1, under these conditions $F : H^{1/2}(\partial D) \to H^{-1/2}(\partial D)$ is self-adjoint, bijective and either positive or negative definite. In what follows, we will denote by $|F|$ the absolute value of F, meaning that $|F| = F$ if F is positive, and $|F| = -F$ if F is negative. The following lemma, like most of the content of this section, is adopted from [4].

Lemma 6.1. *The operator $|F| : H^{1/2}(\partial D) \to H^{-1/2}(\partial D)$ can be given as $|F| = (F^{1/2})' F^{1/2}$, where $F^{1/2} : H^{1/2}(\partial D) \to L^2(\partial D)$ and $(F^{1/2})' : L^2(\partial D) \to H^{-1/2}(\partial D)$ are bounded, bijective and dual to each other.*

By using theorem 4.1 and lemma 6.1, it is easy to see that the absolute value of the difference of the Robin-to-Robin boundary maps, defined by

$$|\Upsilon - \Upsilon_0| = L|F|L' = L(F^{1/2})' F^{1/2} L' : H^{-1/2}(\partial\Omega) \to H^{1/2}(\partial\Omega), \qquad (6.1)$$

is positive definite. As a consequence, the unique, positive, restricted square root operator $|\Upsilon - \Upsilon_0|^{1/2}_{L^2(\partial\Omega)} : L^2(\partial\Omega) \to L^2(\partial\Omega)$ is well defined. The following lemma is a straightforward consequence of the factorization (6.1)—for proof we refer again to [4].

Lemma 6.2. *The ranges $\mathcal{R}\big(|\Upsilon - \Upsilon_0|^{1/2}_{L^2(\partial\Omega)}\big)$ and $\mathcal{R}(L)$ coincide.*

Note that $\mathcal{R}\big(|\Upsilon - \Upsilon_0|^{1/2}_{L^2(\partial\Omega)}\big)$ is something that can be obtained through boundary measurements and, as a consequence, so is $\mathcal{R}(L)$. Keeping this in mind, we consider the solution h_y of the following homogeneous Robin problem:

$$\begin{aligned} &\nabla \cdot K_0 \nabla h(x) - \mu_0 h(x) = \delta(x - y) \qquad \text{in } \Omega, \\ &\gamma h + \tfrac{1}{2}\nu \cdot K_0 \nabla h = 0 \qquad \text{on } \partial\Omega, \end{aligned} \qquad (6.2)$$

where $y \in \Omega$ is a parameter and δ is the delta functional. Physically speaking, h_y is the energy fluency corresponding to a point source at y and no input flux on $\partial\Omega$. It is well known that (6.2) is uniquely solvable with $h_y \in C^\infty(\Omega \backslash \{y\})$ and h_y singular at y.

Now it is the time to present the main result of this work. Note that the algorithm induced by the following theorem is non-invasive: Υ_0 and h_y can be computed and Υ can be measured.

Theorem 6.3. *Let $K_0, \mu_0 \in C^\infty(\Omega)$ and $\kappa, \delta \in C^\infty(\overline{D})$ be scalar functions and assume that either (5.1) holds and κ is negative on ∂D or (5.2) is valid and κ is positive on ∂D. Then the output flux $\big(\gamma h_y - \frac{1}{2}\nu \cdot K_0 \nabla h_y\big)\big|_{\partial\Omega}$, corresponding to the singular solution of (6.2), belongs to the range of $|\Upsilon - \Upsilon_0|^{1/2}_{L^2(\partial\Omega)}$ if and only if $y \in D$.*

Proof. Let us first consider the case $y \in D$. Since $h_y|_{\Omega\backslash D}$ is smooth, it is easy to see that it is the unique solution of (4.2) corresponding to $\Psi = \big(\gamma h_y + \frac{1}{2}\nu \cdot K_0 \nabla h_y\big)^-\big|_{\partial D}$. In other words,

$$L\Big(\big(\gamma h_y + \tfrac{1}{2}\nu \cdot K_0 \nabla h_y\big)^-\big|_{\partial D}\Big) = \big(\gamma h_y - \tfrac{1}{2}\nu \cdot K_0 \nabla h_y\big)\big|_{\partial\Omega},$$

which proves one part of the claim.

To prove the other part, we assume the opposite: Let $y \in \Omega\backslash D$ and $\Psi \in H^{-1/2}(\partial D)$ be such that the solution of (4.2) satisfies $\gamma v - \frac{1}{2}\nu \cdot K_0 \nabla v = \gamma h_y - \frac{1}{2}\nu \cdot K_0 \nabla h_y$ on $\partial\Omega$. Due to the outer boundary conditions of (4.2) and (6.2), v and h_y have the same Cauchy data on $\partial\Omega$, and so it follows from Holmgren's uniqueness theorem that $v = h_y$ on $\Omega\backslash(\overline{D} \cup \{y\})$. Since h_y is singular at y whereas v is not, we have arrived at a contradiction, which completes the proof. □

In theorem 6.3, the behaviour of the diffusion tensor is more important than the behaviour of the absorption coefficient since a strict inequality is posed only on κ. In consequence, the factorization method is applicable to the characterization of purely diffusive inclusions whereas there is no guarantee that it would work for purely absorbing inhomogeneities.

To end this work, we note that the above theorem can be generalized for the case of multiple non-intersecting inclusions, $D_1, \ldots, D_m \subset \Omega$, by replacing the trace spaces $H^{\pm 1/2}(\partial D)$ used above with the products $H^{\pm 1/2}(\partial D_1) \times \cdots \times H^{\pm 1/2}(\partial D_m)$. The numerical implementation of theorem 6.3 will be considered in forthcoming papers.

References

[1] Arridge S R 1999 Optical tomography in medical imaging *Inverse Problems* **15** R41–93

[2] Arridge S R 2002 Diffusion tomography in dense media *Scattering: Scattering and Inverse Scattering in Pure and Applied Science* vol 1 ed R Pike and P Sabatier (London: Academic) pp 920–36

[3] Arridge S R and Hebden J C 1997 Optical imaging in medicine: II. Modelling and reconstruction *Phys. Med. Biol.* **42** 841–53

[4] Brühl M 2001 Explicit characterization of inclusions in electrical impedance tomography *SIAM J. Math. Anal.* **32** 1327–41

[5] Case K M and Zweifel P F 1967 *Linear Transport Theory* (New York: Addison-Wesley)

[6] Dautray R and Lions J-L 1988 *Mathematical Analysis and Numerical Methods for Science and Technology* vol 2 (Berlin: Springer)

[7] Hebden J C, Arridge S R and Delpy D T 1997 Optical imaging in medicine: I. experimental techniques *Phys. Med. Biol.* **42** 825–40

[8] Heino J and Somersalo E 2002 Estimation of optical absorption in anisotropic background *Inverse Problems* **18** 559–73

[9] Hyvönen N 2002 Analysis of optical tomography with non-scattering regions *Proc. Edinburgh Math. Soc.* **45** 257–76

[10] Hyvönen N 2004 Complete electrode model of electrical impedance tomography: approximation properties and characterization of inclusions *SIAM J. Appl. Math.* at press

[11] Kirsch A 1998 Characterization of the shape of the scattering obstacle using the spectral data of the far field operator *Inverse Problems* **14** 1489–512

[12] Ladyzhenskaya O A 1985 *The Boundary Value Problems of Mathematical Physics* (New York: Springer)

[13] Taylor M E 1996 *Partial Differential Equations I* (New York: Springer)

[14] Yosida K 1980 *Functional Analysis* 6th edn (New York: Springer)