

# On uniqueness in diffuse optical tomography

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## **Abstract.**

A prominent result of Arridge and Lionheart (1998 *Opt. Lett.* **23** 882–4) demonstrates that it is in general not possible to simultaneously recover both the diffusion (aka scattering) and the absorption coefficient in steady-state (dc) diffusion-based optical tomography. In this work we show that it suffices to restrict ourselves to piecewise constant diffusion and piecewise analytic absorption coefficients to regain uniqueness. Under this condition both parameters can simultaneously be determined from complete measurement data on an arbitrarily small part of the boundary.

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## 1. Introduction

We consider the following inverse problem. Determine *simultaneously* the real-valued diffusion (aka scattering) and absorption coefficients,  $a(x)$  and  $c(x)$ , of the elliptic partial differential equation

$$-\nabla \cdot (a\nabla u) + cu = 0 \quad \text{in } B \quad (1)$$

from knowledge of all possible pairs of Neumann and Dirichlet boundary values,  $a\partial_\nu u|_S$  and  $u|_S$ , on an arbitrarily small open part  $S$  of the boundary  $\partial B$  of some domain  $B \subset \mathbb{R}^n$ ,  $n \geq 2$ , with outer normal  $\nu$ .

This problem arises in steady-state (dc) diffusion based optical tomography, where light propagation is modeled by a diffusion approximation and the excitation frequency is set to zero. For a full description of optical tomography including the derivation of (1) we refer the reader to the topical reviews of Arridge [2] and Gibson, Hebden and Arridge [8].

A prominent result by Arridge and Lionheart [3] demonstrates that this inverse problem is in general not uniquely solvable, i.e., it is not possible to uniquely determine both  $a$  and  $c$  from boundary data of  $u$ . The reason is that a diffusion coefficient can be transformed into an absorption coefficient by setting

$$v := \sqrt{a}u$$

which transforms (1) into

$$-\Delta v + \eta v = 0, \quad \eta = \frac{\Delta\sqrt{a}}{\sqrt{a}} + \frac{c}{a}. \quad (2)$$

If  $a = 1$  in a neighborhood of  $\partial B$  then the boundary values remain unchanged. Hence, boundary measurements can only contain information about  $\eta$ , from which one cannot extract  $a$  and  $c$ .

Despite this negative theoretical result, several experimental works succeeded in the simultaneous reconstruction of diffusion and absorption properties, see the references in [8, section 3.4.3]. This apparent conflict between theoretical and practical results is explained by the fact that every reconstruction algorithm incorporates prior information in some form, e.g. by regularizing the underlying ill-posed problem. It is therefore desirable to develop a deeper understanding of the degree of non-uniqueness in optical tomography and to identify (preferably weak) prior information that lead to uniqueness.

In this work we show that uniqueness holds for piecewise constant diffusion and piecewise analytic absorption coefficients. We prove that under this condition both parameters are simultaneously uniquely determined by knowledge of all possible pairs of Neumann and Dirichlet boundary values  $a\partial_\nu u|_S$ ,  $u|_S$  of solutions  $u$  of (1), see theorem 4.2. We also comment on the consequences of our result to the much discussed question up to what extent dc optical tomography can differentiate between diffusion and absorption effects, cf section 5.

The main tool for our uniqueness proof is the technique of localized potentials developed by the author in [6]. Localized potentials are solutions of (1) that are large

on some specified subset of the domain  $B$  while staying small on other subsets. The idea of using growth properties of special solutions is widely spread in the study of coefficient determination problems for partial differential equations; cf Kohn and Vogelius [14, 15], Isakov [12], Alessandrini [1], Nachman [19], and Sylvester and Uhlmann [21], to name just a few of the seminal works that seeded this idea in the mathematical community. The specialty of the localized potentials used here is that their construction relies on abstract, but simple, functional analytic arguments, which makes them quite adaptable to different situations. Notably, we adapt them in this work to (up to some obvious limits) independently control the solutions'  $H^1$ - and  $L^2$ -norms on specific subsets. This enables us to show with a simple monotony argument that the boundary measurements determine first the diffusion and then also the absorption coefficient.

To the author's knowledge the present work is the first result on simultaneous uniqueness for a class of real-valued diffusion and absorption coefficients. A characterization of the combined support of diffusive and absorbing inclusions can be found in [7]. Also, if  $a$  is real but  $c$  has a known, non-zero imaginary part then one can reconstruct  $\eta$  in (2) and extract  $c$  and  $a$  from it, cf Grinberg [9]. A recent numerical study of Hein and Meyer [10] treats the identification of  $a$  and  $c$  from interior data measured everywhere in  $B$ . Some results on the simultaneous recovery of convection and absorption coefficients and results in the context of Maxwell's and elasticity equations are summarized in the book of Isakov [13].

The outline of this paper is as follows. We start with a more detailed description of the considered problem in section 2. Then we derive the existence of localized potentials for diffuse optical tomography in section 3. In section 4 we formulate and prove our main result on the simultaneous determinability of diffusion and absorption coefficients. The consequences of our result are discussed in section 5 which also contains some concluding remarks.

## 2. Diffuse optical tomography

We start with a more detailed description of the considered problem. Let  $B \subset \mathbb{R}^n$ ,  $n \geq 2$ , be a bounded domain with piecewise smooth boundary  $\partial B$  describing the medium that is to be imaged (see definition 2.1 below for our definition of a piecewise smooth boundary). We assume that the propagation of light through this medium can be modeled by the steady-state diffusion approximation

$$-\nabla \cdot (a\nabla u) + cu = 0 \quad \text{in } B, \quad (3)$$

where  $u : B \rightarrow \mathbb{R}$  describes the photon density in the medium,  $a : B \rightarrow \mathbb{R}$  is the isotropic diffusion and  $c : B \rightarrow \mathbb{R}$  the absorption coefficient, cf the reviews on optical tomography cited in the introduction.

We furthermore assume that boundary measurements of inward and outward light fluxes give us access to the Neumann and Dirichlet boundary values of all solutions of (3) on an open and smooth piece  $S$  of the boundary. For ease of presentation we model

the rest of the boundary  $\partial B \setminus \overline{S}$  by a homogeneous Neumann boundary condition. Thus, the boundary measurements determine the local Neumann-to-Dirichlet operator

$$\Lambda_{a,c} : g \mapsto u|_S, \quad (4)$$

where  $u$  solves

$$-\nabla \cdot (a\nabla u) + cu = 0 \quad \text{in } B, \quad a\partial_\nu u|_{\partial B} = \begin{cases} g & \text{on } S, \\ 0 & \text{elsewhere.} \end{cases} \quad (5)$$

If  $a, c \in L^{\infty}_+(B)$ , where the subscript “+” denotes positive essential infima, then it follows from the variational formulation of (5), the Lax-Milgram theorem (cf, e.g. Dautray and Lions [4, VI, §3, Thm. 7]), and Sobolev trace and embedding theorems (cf, e.g. Taylor [22, Chp. 4, Prop. 4.4, 4.5]), that equation (5) possesses a unique solution  $u \in H^1(B)$  for all  $g \in L^2(S)$ , and that  $\Lambda_{a,c}$  is a linear, compact and self-adjoint operator from  $L^2(S)$  to  $L^2(S)$ .

Let us note that this is a very simplified way of modeling boundary measurements in diffuse optical tomography. More realistic approaches model light sources as point sources located at a small depth below the surface  $\partial B$ , or by a Robin boundary condition (cf, e.g. Arridge [2, Sect. 3.5] and Heino and Somersalo [11]). Also, the measured outward light flux should rather be modeled by a Robin boundary condition, possibly including the effects of boundary reflection.

However, we believe that our simple boundary model already contains the essential aspects for the theoretical study of unique simultaneous determinability of  $a$  and  $c$ . For  $S = \partial B$  it agrees with the setting for which Arridge and Lionheart have derived their non-uniqueness example. Also, for  $S = \partial B$ , knowledge of a Robin-to-Robin mapping is usually equivalent to knowing the Neumann-to-Dirichlet operator as long as there are no additional unknown coefficients in the Robin conditions. For  $S \subsetneq \partial B$  this equivalence is no longer true due to the homogeneous Neumann boundary condition on  $\partial B \setminus \overline{S}$ , but we are confident that our arguments can be modified to hold also for other types of boundary conditions on  $\partial B \setminus \overline{S}$ .

Our uniqueness result holds for *piecewise constant* diffusivities  $a$  and *piecewise analytic* absorption coefficients  $c$ . We finish this section by making these assumptions precise.

**Definition 2.1.** (a) An open set  $O$  is said to have a smooth boundary if  $\partial O$  is locally a  $C^\infty$  curve, and  $O$  lies locally on one side of  $\partial O$ .

(b) An open set  $O$  is said to have a piecewise smooth boundary if  $\partial O$  is a countable union of  $C^\infty$  curves, and  $O$  lies locally on one side of  $\partial O$ .

(c) A function  $a \in L^\infty(B)$  is called piecewise constant if there exists finitely many pairwise disjoint subdomains  $O_1, \dots, O_m \subset B$  with piecewise smooth boundaries, such that  $\overline{B} = \overline{O_1 \cup \dots \cup O_m}$  and  $a|_{O_j}$  is constant,  $j = 1, \dots, m$ .

(d) A function  $c \in L^\infty(B)$  is called piecewise analytic if there exists finitely many pairwise disjoint subdomains  $O_1, \dots, O_m \subset B$  with piecewise smooth boundaries,

such that  $\overline{B} = \overline{O_1 \cup \dots \cup O_m}$ , and  $c|_{O_j}$  has an extension which is analytic in a neighborhood of  $\overline{O_j}$ ,  $j = 1, \dots, m$ .

### 3. Localized potentials for optical tomography

#### 3.1. Intuitive ideas

The main tool for our uniqueness proof is the technique of localized potentials developed by the author in [6]. Roughly speaking, localized potentials mean photon densities  $u$  that are large on some specified subset of the domain  $B$  while staying small outside this subset. For the case that  $c = 0$  in equation (5) which then describes electrical impedance tomography, [6, Thm 2.7] shows that such potentials exist for almost arbitrary subsets as long as they can be connected to the boundary. Here we do not only extend this result to equation (5) with  $c > 0$ , but also show that (up to some extent) we can independently control the  $H^1$ -norm  $\|u\|_{H^1}$  and the  $L^2$ -norm  $\|u\|_{L^2}$  of solutions of (5).

We begin with a somewhat loose, intuitive description of the general ideas behind this technique. For rigorous formulations and proofs of the following arguments we refer the reader to theorem 3.1 and its proof.

The existence of localized potentials is derived from a *duality principle* between source terms added to the right hand side of the diffusion equation (3) (with homogeneous Neumann boundary conditions) and the effect of these source terms on a source-free solution of (5).

To give an idea of this duality, consider a monopole (delta) source  $\delta_z$  located in a point  $z$  added to the right hand side of (3). The dual of this source would be the effect of a delta source on a (source-free) solution  $u$  of (5), i.e. the evaluation  $u(z)$ . Likewise the dual of a dipole source term  $d \cdot \nabla \delta_z$  in some direction  $d \in \mathbb{R}^n$  is the evaluation of the gradient  $d \cdot \nabla u(z)$ . The dual of monopole densities on some subset  $O$  is the  $L^2$ -norm of  $u|_O$  restricted to this subset, and the dual of dipole densities on  $O$  is the  $L^2$ -norm of  $\nabla u|_O$ , i.e. essentially the  $H^1$ -norm of  $u$  on  $O$ . Rigorously, these dualities can be formulated in terms of bounded linear operators between Hilbert spaces, cf the beginning of the proof of theorem 3.1.

Now a functional analytic principle asserts that if one source is able to generate some boundary data that another one cannot produce, then the dual quantity of the first source can not be bounded by that of the other source. In other words, if there exist boundary values that, e.g., can only be explained by a collection of monopole sources on some subset  $O_1$  but not by monopole sources on some other subset  $O_2$ , then there exist solutions of (5) with very large ( $L^2$ -)norm on  $O_1$  but very small ( $L^2$ -)norm on  $O_2$ . For a rigorous formulation of the functional analytic principle we refer again to the proof of theorem 3.1, or to the therein cited [6, Lemma 2.5].

To apply this principle, consider the situation sketched on the upper left side of figure 1. Assume that there are dipole sources located on the dark grey complement  $B \setminus \overline{O}$  of the white neighborhood  $O$  of the boundary piece  $S$ . Since  $S$  has some distance

from  $B \setminus \overline{O}$ , the effect of these sources on measurements on  $S$  will be somewhat smoothed. Thus, such sources cannot give rise to all the boundary measurements on  $S$  that sources on  $O$  can create. Likewise, dipole sources on  $O$  can create less smooth measurements on  $S$  than monopole sources can. From the duality principle we therefore obtain that (by applying the right optical fluxes on  $S$ ) we can make the  $H^1$ -norm of the resulting photon density  $u$  arbitrarily large on  $O$  while keeping its  $L^2$ -norm on  $O$  as well as its  $H^1$ -norm outside  $O$  small. Note, that it is essential for these arguments that  $O$  is connected with the boundary part  $S$ .

In the situation sketched on the lower left of figure 1, it is due to unique continuation that (monopole) sources on the white subset  $O'$  of  $O$  can give rise to measurements that (dipole) sources on the dark grey complement  $B \setminus \overline{O}$  cannot create. Hence, we can construct a photon density with arbitrarily large  $L^2$ -norm on the subset  $O'$  of  $O$ , and arbitrarily small  $H^1$ -norm outside  $O$ . Note that this time it is essential for the unique continuation argument that there exists the light grey domain  $O \setminus \overline{O'}$  that connects  $O'$  as well as  $B \setminus \overline{O}$  with the boundary piece  $S$ .

We can also combine unique continuation with smoothness arguments to treat the situation on the upper right of figure 1. There, we can make the  $H^1$ -norm of a photon density blow up in the interior subdomain  $\Omega$ , without blowing up its  $L^2$ -norm on  $\Omega$  or its  $H^1$ -norm outside  $\Omega$  and some domain  $O$  that connects it to the boundary  $S$ . Again, we can also make its  $L^2$ -norm blow up on a subset  $\Omega'$  of  $\Omega$  without blowing up its  $H^1$ -norm outside  $\overline{\Omega \cup O}$ , cf the lower right of figure 1.

In section 4, we will use these localized potentials to show that deviations in the diffusion or absorption coefficients lead to deviations in the measurements. A detailed description will be given there.

### 3.2. Existence of localized potentials

We now rigorously state and prove our existence result on localized potentials.

**Theorem 3.1.** *Let  $a, c \in L_+^\infty(B)$  be piecewise analytic. Let  $O$  be a subdomain of  $B$ , for which  $S$  is a smooth part of the boundary  $\partial O$ .*

- (a) (i) *There exists a sequence  $(g_k)_{k \in \mathbb{N}} \subset L^2(S)$  such that the corresponding solutions  $(u_k)_{k \in \mathbb{N}} \subset H^1(B)$  of equation (5) satisfy*

$$\|u_k\|_{H^1(O)} \rightarrow \infty, \quad \|u_k\|_{L^2(O)} \rightarrow 0, \quad \|u_k\|_{H^1(B \setminus \overline{O})} \rightarrow 0;$$

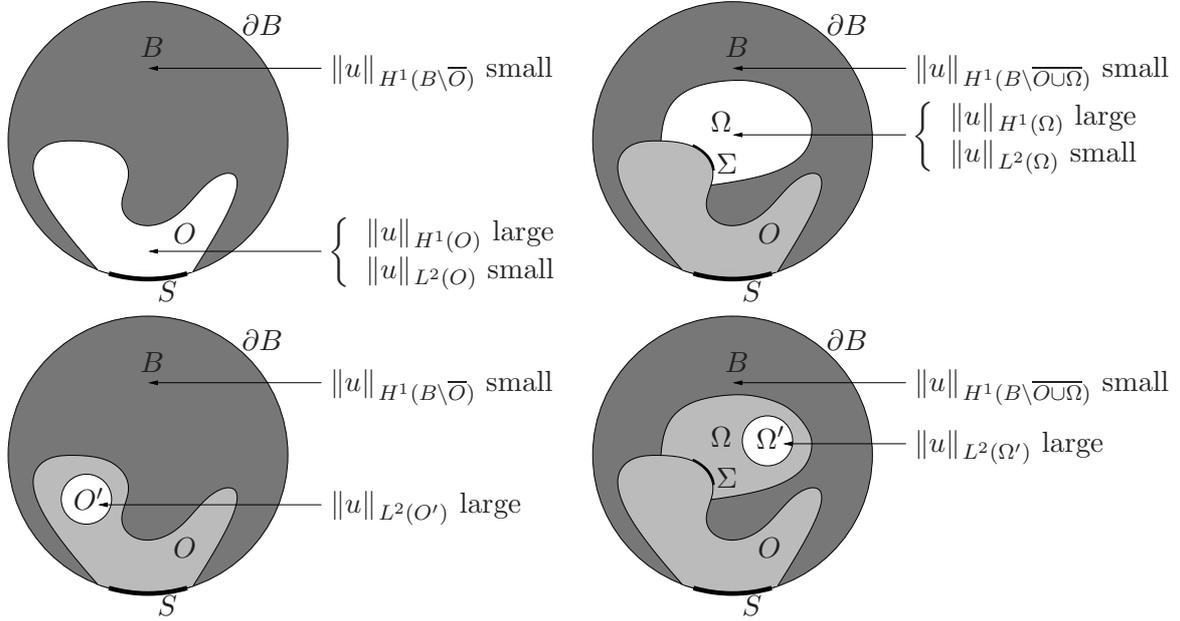
*cf the upper left picture in figure 1.*

- (ii) *Let  $O'$  be an open subset of  $O$ . There exist  $(g_k)_{k \in \mathbb{N}} \subset L^2(S)$  such that the corresponding solutions  $(u_k)_{k \in \mathbb{N}} \subset H^1(B)$  of equation (5) satisfy*

$$\|u_k\|_{L^2(O')} \rightarrow \infty, \quad \|u_k\|_{H^1(B \setminus \overline{O})} \rightarrow 0;$$

*cf the lower left picture in figure 1.*

- (b) *Let  $\Omega$  be another open subset of  $B$ , with  $\Omega \cap O = \emptyset$ , and let  $\partial\Omega$  and  $\partial O$  contain a joint smooth open piece  $\Sigma$ .*



**Figure 1.** Sketch of the localized potentials constructed in theorem 3.1

- (i) There exists a sequence  $(g_k)_{k \in \mathbb{N}} \subset L^2(S)$  such that the corresponding solutions  $(u_k)_{k \in \mathbb{N}} \subset H^1(B)$  of equation (5) satisfy

$$\|u_k\|_{H^1(\Omega)} \rightarrow \infty, \quad \|u_k\|_{L^2(\Omega)} \rightarrow 0, \quad \|u_k\|_{H^1(B \setminus \overline{O \cup \Omega})} \rightarrow 0;$$

of the upper right picture in figure 1.

- (ii) Let  $\Omega'$  be an open subset of  $\Omega$ . There exist  $(g_k)_{k \in \mathbb{N}} \subset L^2(S)$  such that the corresponding solutions  $(u_k)_{k \in \mathbb{N}} \subset H^1(B)$  of equation (5) satisfy

$$\|u_k\|_{L^2(\Omega')} \rightarrow \infty, \quad \|u_k\|_{H^1(B \setminus \overline{O \cup \Omega})} \rightarrow 0;$$

of the lower right picture in figure 1.

### 3.3. Proof of theorem 3.1

We first note the following unique continuation property. For every open connected subset  $U \subseteq B$  only the trivial solution of

$$-\nabla \cdot (a \nabla u) + cu = 0 \quad \text{in } U,$$

vanishes on an open subset of  $U$  or possesses zero Cauchy data on a smooth, open part of  $\partial U$ . For Lipschitz continuous  $a$  and bounded  $c$ , this property is proven in Miranda [18, Thm. 19, II]. It can be extended to our case of piecewise analytic  $a$  and  $c$  by sequentially solving Cauchy problems (see also Druskin [5] for this argument).

Now we apply the ideas of [6] and rewrite the assertion using a functional analytic relation between the norm of an operator and the range of its adjoint. To this end we introduce the solution operator

$$G : H^1(B)' \rightarrow L^2(S), \quad f \mapsto u|_S,$$

where  $u \in H^1(B)$  solves

$$\int_B (a \nabla u \cdot \nabla v + cuv) \, dx = \langle f, v \rangle_B \quad \text{for all } v \in H^1(B). \quad (6)$$

Here and in the following  $\langle \cdot, \cdot \rangle_U$  denotes the dual pairing on  $H^1(U)' \times H^1(U)$  for an open set  $U \subseteq B$ , and if  $U$  is also smoothly bounded then  $\langle \cdot, \cdot \rangle_{\partial U}$  is the dual pairing on  $H^{-1/2}(\partial U) \times H^{1/2}(\partial U)$ .

It is easily checked that the dual operator of  $G$  is given by

$$G' : L^2(S) \rightarrow H^1(B), \quad g \mapsto u,$$

where  $u \in H^1(B)$  solves

$$\int_B (a \nabla u \cdot \nabla v + cuv) \, dx = \int_S gv|_S \, ds \quad \text{for all } v \in H^1(B),$$

i.e.,  $G'$  maps a given Neumann datum  $g$  to the solution  $u \in H^1(B)$  of equation (5).

For open subsets  $U$  of  $B$  we will also use the restriction operator

$$r_U : H^1(B) \rightarrow H^1(U), \quad u \mapsto u|_U,$$

and the compact injection  $\iota_U : H^1(U) \hookrightarrow L^2(U)$ . Their duals are the canonical injections

$$r'_U : H^1(U)' \rightarrow H^1(B)', \quad \langle r'_U f, v \rangle_B = \langle f, v|_U \rangle_U$$

for all  $f \in H^1(U)'$ ,  $v \in H^1(B)$  and

$$\iota'_U : L^2(U) \rightarrow H^1(U)', \quad \langle \iota'_U f, v \rangle_U = \int_U f v \, dx.$$

for all  $f \in L^2(U)$ ,  $v \in H^1(U)$ .

Using these operators the assertion can be written as

(a) (i) There exist  $(g_k)_{k \in \mathbb{N}} \subset L^2(S)$ , such that

$$\|r_O G' g_k\| \rightarrow \infty, \quad \|\iota_O r_O G' g_k\| \rightarrow 0, \quad \|r_{B \setminus \overline{O}} G' g_k\| \rightarrow 0.$$

(ii) There exist  $(g_k)_{k \in \mathbb{N}} \subset L^2(S)$ , such that

$$\|\iota_{O'} r_{O'} G' g_k\| \rightarrow \infty, \quad \|r_{B \setminus \overline{O}} G' g_k\| \rightarrow 0.$$

(b) (i) There exist  $(g_k)_{k \in \mathbb{N}} \subset L^2(S)$ , such that

$$\|r_\Omega G' g_k\| \rightarrow \infty, \quad \|\iota_\Omega r_\Omega G' g_k\| \rightarrow 0, \quad \|r_{B \setminus \overline{O \cup \Omega}} G' g_k\| \rightarrow 0.$$

(ii) There exist  $(g_k)_{k \in \mathbb{N}} \subset L^2(S)$ , such that

$$\|\iota_{\Omega'} r_{\Omega'} G' g_k\| \rightarrow \infty, \quad \|r_{B \setminus \overline{O \cup \Omega}} G' g_k\| \rightarrow 0.$$

For bounded linear operators  $A_j : H_j \rightarrow H$ ,  $j = 1, 2$ , between Hilbert spaces  $H$ ,  $H_1$  and  $H_2$  it holds that

$$\mathcal{R}(A_1) \subseteq \mathcal{R}(A_2), \quad \text{if and only if } \exists C > 0 : \|A'_1 g\| \leq C \|A'_2 g\| \quad \forall g \in H';$$

cf, e.g. [6, Lemma 2.5]. We apply this equivalence using

$$A'_1 := r_O G' : L^2(S) \rightarrow H^1(O), \quad \text{and} \\ A'_2 := \begin{pmatrix} \iota_O r_O G' \\ r_{B \setminus \overline{O}} G' \end{pmatrix} : L^2(S) \rightarrow L^2(O) \times H^1(B \setminus \overline{O}),$$

for the first part of (a), and analogous expressions for the other part of (a) and the two parts of (b). Thus, we obtain that the assertion follows from

- (a) (i) There exist  $h \in L^2(S)$  such that  $h \in Gr'_O(H^1(O)')$ , but  
 $h \notin Gr'_{O'}(L^2(O)) + Gr'_{B \setminus \overline{O}}(H^1(B \setminus \overline{O})')$ .
- (ii) There exist  $h \in L^2(S)$  such that  $h \in Gr'_{O'}(L^2(O'))$ , but  
 $h \notin Gr'_{B \setminus \overline{O}}(H^1(B \setminus \overline{O})')$ .
- (b) (i) There exist  $h \in L^2(S)$  such that  $h \in Gr'_\Omega(H^1(\Omega)')$ , but  
 $h \notin Gr'_{\Omega'}(L^2(\Omega)) + Gr'_{B \setminus \overline{\Omega}}(H^1(B \setminus \overline{\Omega \cup \Omega'})')$ .
- (ii) There exist  $h \in L^2(S)$  such that  $h \in Gr'_{\Omega'}(L^2(\Omega'))$ , but  
 $h \notin Gr'_{B \setminus \overline{\Omega \cup \Omega'}}(H^1(B \setminus \overline{\Omega \cup \Omega'})')$ .

This is what we will show now.

- (a) (i) Let  $U \subseteq O$  be a smoothly bounded open set on which  $a$  and  $c$  are analytic, and  $\partial U \cap S$  contain an open smooth piece  $S'$  with  $\overline{S'} \subset \partial U \cap S$ . For every  $g \in Gr'_{O'}(L^2(O)) + Gr'_{B \setminus \overline{O}}(H^1(B \setminus \overline{O})')$ , we have that  $g|_{S'}$  is the Dirichlet boundary value  $u|_{S'}$  of a solution  $u \in H^1(U)$  of

$$-\nabla \cdot (a \nabla u) + cu = f \quad \text{in } U, \quad a \partial_\nu u|_{S \cap \partial U} = 0$$

with  $f \in L^2(U)$ . Multiplying  $u$  with a smooth cutoff function that is 1 in a neighbourhood of  $S'$ , vanishes outside  $U$  and has vanishing Neumann-boundary values on  $\partial U$ , we obtain from standard regularity results (cf, e.g. Dautray and Lions [4, VII, §3, Thm. 2]) that  $u \in H^2(U)$ . Hence  $g|_{S'} = u|_{S'} \in H^{3/2}(S')$ , so that we have shown that (the restrictions to  $S'$  of) functions in

$$Gr'_{O'}(L^2(O)) + Gr'_{B \setminus \overline{O}}(H^1(B \setminus \overline{O})')$$

belong to  $H^{3/2}(S')$ .

Now choose a  $h \in H^{1/2}(S)$  that is compactly supported in  $S'$  and that fulfills  $h|_{S'} \notin H^{3/2}(S')$ . From the above arguments we know that

$$h \notin Gr'_{O'}(L^2(O)) + Gr'_{B \setminus \overline{O}}(H^1(B \setminus \overline{O})').$$

However, there exists  $u \in H^1(B)$  with  $u|_S = h$  and  $u$  vanishes outside  $O$ . We define  $f \in H^1(O)'$  by setting

$$\langle f, v \rangle_O := \int_O (a \nabla u \cdot \nabla v + cuv) \, dx \quad \text{for all } v \in H^1(O).$$

Then we obtain for all  $v \in H^1(B)$

$$\begin{aligned} \langle r'_O f, v \rangle_B &= \langle f, v|_O \rangle_O = \int_O (a \nabla u \cdot \nabla v + cuv) \, dx \\ &= \int_B (a \nabla u \cdot \nabla v + cuv) \, dx, \end{aligned}$$

so that  $u$  solves (6) in the definition of  $Gr'_O f$ .

Hence,  $h = Gr'_O f \in Gr'_O(H^1(O)')$  and the first part of (a) is proven.

- (ii) The second part of (a) follows from similar arguments as in [6]. Without loss of generality we can choose  $O'$  so small that  $O \setminus \overline{O'}$  is connected. Then a standard application of unique continuation, cf, e.g. [6, Lemma 2.3] shows that

$$Gr'_{O'\iota'_{O'}}(L^2(O')) \cap Gr'_{B \setminus \overline{O'}}(H^1(B \setminus \overline{O}')) = \{0\}.$$

Also, by unique continuation,  $\iota_{O'}r_{O'}G'$  is injective. Hence,  $Gr'_{O'\iota'_{O'}}(L^2(O'))$  is dense in  $L^2(S)$ , and thus, a fortiori,  $Gr'_{O'\iota'_{O'}}(L^2(O')) \neq \{0\}$ .

Any  $0 \neq h \in Gr'_{O'\iota'_{O'}}(L^2(O'))$  fulfills  $h \notin Gr'_{B \setminus \overline{O'}}(H^1(B \setminus \overline{O}'))$ , so (a)(ii) is proven.

- (b) (i) To show (b)(i), let  $U$  be a smoothly bounded open set, so that  $\overline{U} \subset O \cup \Omega \cup \Sigma$ ,  $U_\Omega := U \cap \Omega$  has a smooth boundary,  $a$  and  $c$  are analytic on  $U_O := U \cap O$  and  $U_\Omega$ , and so that  $U$  contains a smooth open piece  $\Sigma'$  with  $\overline{\Sigma'} \subset \Sigma$ .

We first introduce the operator  $\Gamma$  which is defined in the same way as  $G$  but takes the trace of  $u$  on  $\Sigma'$  rather than on  $S$ , i.e.,

$$\Gamma : H^1(B)' \rightarrow L^2(\Sigma'), \quad f \mapsto u|_{\Sigma'}$$

where  $u \in H^1(B)$  solves (6).

If

$$Gr'_\Omega(H^1(\Omega)') \subseteq Gr'_{\Omega'\iota'_\Omega}(L^2(\Omega)) + Gr'_{B \setminus \overline{O \cup \Omega}}(H^1(B \setminus \overline{O \cup \Omega}'))$$

was true, then by unique continuation on  $O$ , we would obtain that

$$\Gammar'_\Omega(H^1(\Omega)') \subseteq \Gammar'_{\Omega'\iota'_\Omega}(L^2(\Omega)) + \Gammar'_{B \setminus \overline{O \cup \Omega}}(H^1(B \setminus \overline{O \cup \Omega}')).$$

Thus, for the first assertion of (b), it suffices to show that this is not the case. The space  $\Gammar'_{\Omega'\iota'_\Omega}(L^2(\Omega)) + \Gammar'_{B \setminus \overline{O \cup \Omega}}(H^1(B \setminus \overline{O \cup \Omega}'))$  consists only of Dirichlet boundary values  $u|_{\Sigma'}$  of solutions of the diffraction problem

$$-\nabla \cdot (a\nabla u) + cu = f \quad \text{in } U, \quad \text{and} \quad [a\partial_\nu u]_{\Sigma \cap U} = 0,$$

with  $f \in L^2(U)$ . We orient the normal  $\nu$  to point inside  $U_\Omega$ , and denote by  $[a\partial_\nu u]_{\Sigma \cap U} := a\partial_\nu u^+|_{\Sigma \cap U} - a\partial_\nu u^-|_{\Sigma \cap U}$  the difference of the Neumann trace taken from  $U_\Omega$  (denoted by the superscript "+") and the one taken from  $U_O$  (denoted by the superscript "-").

Again, we can multiply  $u$  with a  $C^\infty$ -cutoff function that is equal to one in a neighbourhood of  $\Sigma'$ , vanishes outside  $U$  and has vanishing Neumann boundary values on  $\Sigma \cap U$ . Thus, we can apply regularity results for diffraction problems (cf, e.g., the proof of theorem 16.1 in Ladyzhenskaya and Ural'tseva [16]) to obtain that  $u|_{U_\Omega} \in H^2(U_\Omega)$ . It follows that  $u|_{\Sigma'} \in H^{3/2}(\Sigma')$ , and thus

$$\Gammar'_{\Omega'\iota'_\Omega}(L^2(\Omega)) + \Gammar'_{B \setminus \overline{O \cup \Omega}}(H^1(B \setminus \overline{O \cup \Omega}')) \subseteq H^{3/2}(\Sigma').$$

Now let  $h \in H^{1/2}(\Sigma') \setminus H^{3/2}(\Sigma')$  be compactly supported in  $\Sigma'$ . Then there exists  $u \in H^1(U_\Omega)$  with  $u|_{\Sigma'} = h$ . We then solve the exterior Dirichlet problem on  $B \setminus \overline{U_\Omega}$  with Dirichlet data  $u|_{\partial U_\Omega}$  on  $\partial U_\Omega$  and zero Neumann condition on  $\partial B$  to extend  $u$  to a function on  $B$  with

$$-\nabla \cdot (a\nabla u) + cu = 0 \quad \text{in } B \setminus \overline{U_\Omega} \tag{7}$$

and  $a\partial_\nu u|_{\partial B} = 0$ . The extended function  $u$  fulfills

$$u|_{U_\Omega} \in H^1(U_\Omega), \quad u|_{B \setminus \overline{U_\Omega}} \in H^1(B \setminus \overline{U_\Omega}),$$

and  $u^+|_{\partial U_\Omega} = u^-|_{\partial U_\Omega}$ , where the superscripts ”+”, resp ”-”, denote that the trace is taken from  $U_\Omega$ , resp. from  $B \setminus \overline{U_\Omega}$ . Hence,  $u \in H^1(B)$ . Furthermore, since  $u$  solves (7), it has a well defined Neumann trace  $a\partial_\nu u^-|_{\partial U_\Omega} \in H^{-1/2}(\partial U_\Omega)$ , taken from  $B \setminus \overline{U_\Omega}$ .

We define  $f \in H^1(\Omega)'$  by setting for all  $v \in H^1(\Omega)$

$$\langle f, v \rangle_\Omega := \int_{U_\Omega} (a\nabla u \cdot \nabla v + cuv) \, dx + \langle a\partial_\nu u^-|_{\partial U_\Omega}, v|_{\partial U_\Omega} \rangle_{\partial U_\Omega}.$$

Then,

$$\begin{aligned} \langle r'_\Omega f, v \rangle_B &= \langle f, v|_\Omega \rangle_\Omega \\ &= \int_{U_\Omega} (a\nabla u \cdot \nabla v + cuv) \, dx + \langle a\partial_\nu u^-|_{\partial U_\Omega}, v|_{\partial U_\Omega} \rangle_{\partial U_\Omega} \\ &= \int_B (a\nabla u \cdot \nabla v + cuv) \, dx, \end{aligned}$$

so that  $u$  solves (6) in the definition of  $\Gamma r'_\Omega f$ .

Hence,  $h = u|_{\Sigma'} = \Gamma r'_\Omega f \in \Gamma r'_\Omega(H^1(O)')$  and (b)(i) is proven.

- (ii) The second part of (b) follows from the same arguments that we used for the second part of (a).  $\square$

## 4. Simultaneous recovery of diffusion and absorption

### 4.1. The main result

We will now apply the localized potentials from the last section to show that both the diffusion coefficient  $a$ , and the absorption coefficient  $c$ , can simultaneously be determined by complete boundary measurements, i.e., the local Neumann-to-Dirichlet operator  $\Lambda_{a,c}$ , on an arbitrarily small, smooth and open part  $S$  of the boundary, cf section 2 for the definition of  $\Lambda_{a,c}$ . The connection between localized potentials and the uniqueness question comes from the following simple monotony relation.

**Lemma 4.1.** *Let  $a_1, a_2, c_1, c_2 \in L_+^\infty(B)$ . Then*

$$\begin{aligned} \int_B ((a_2 - a_1)|\nabla u_1|^2 + (c_2 - c_1)|u_1|^2) \, dx & \quad (8) \\ \geq \langle (\Lambda_{a_1, c_1} - \Lambda_{a_2, c_2})g, g \rangle & \geq \int_B ((a_2 - a_1)|\nabla u_2|^2 + (c_2 - c_1)|u_2|^2) \, dx, \end{aligned}$$

for all  $g \in L^2(S)$  where  $u_1, u_2 \in H^1(B)$  are the solutions of (5) with Neumann boundary data  $g$  on  $S$ , and coefficients  $(a_1, c_1)$ , resp.,  $(a_2, c_2)$ .

*Proof.* This can be shown analogously to e.g. [6, Lemma 3.1]. Since the order of the terms is easily mixed up, we also give a proof in the appendix.  $\square$

The consequence of Lemma 4.1 is that we can control the quadratic form

$$\langle (\Lambda_{a_1, c_1} - \Lambda_{a_2, c_2})g, g \rangle \quad (9)$$

by controlling either  $|\nabla u_2|^2$  or  $|u_2|^2$  on subdomains of  $B$ . To explain this argument more precisely, let us first assume that  $a_2 > a_1$  in some neighborhood of  $S$ . Then let  $g$  be a Neumann datum creating a localized potential  $u_2$  with large  $|\nabla u_2|^2$  but small  $|u_2|^2$  in this neighborhood and also small  $|\nabla u_2|^2$  outside this neighborhood. This will make the right hand side of (8), and thus the quadratic form (9) very large, so that in particular  $\Lambda_{a_1, c_1} \neq \Lambda_{a_2, c_2}$ .

On the other hand, if  $a_1 = a_2$  but  $c_2 > c_1$  in a neighborhood of  $S$  then a localized potential with large  $|u_2|^2$  in this neighborhood and small  $|\nabla u_2|^2$  outside, will make the quadratic form large. The same kind of arguments can be used for the case that  $a_2 > a_1$  or  $c_2 > c_1$  somewhere in the interior of  $B$  by using the localized potentials from part (b) of theorem 3.1, and, of course, also after interchanging  $(a_2, c_2)$  and  $(a_1, c_1)$ .

Thus, we can make the absolute value of the quadratic form  $|\langle (\Lambda_{a_1, c_1} - \Lambda_{a_2, c_2})g, g \rangle|$  large, whenever  $(a_1, c_1)$  and  $(a_2, c_2)$  are different pairs of piecewise constant coefficients. Using the fact that we can make the  $L^2$ -norm of the localized potentials large in every subset of the considered neighborhoods, the arguments extend to piecewise analytic absorption coefficients. In all cases, it follows that  $\Lambda_{a_1, c_1} \neq \Lambda_{a_2, c_2}$ .

From these intuitive arguments we obtain our main result.

**Theorem 4.2.** *Let  $a_1, a_2 \in L_+^\infty(B)$  be piecewise constant and  $c_1, c_2 \in L_+^\infty(B)$  be piecewise analytic. If  $\Lambda_{a_1, c_1} = \Lambda_{a_2, c_2}$  then*

$$a_1 = a_2 \quad \text{and} \quad c_1 = c_2.$$

#### 4.2. Proof of theorem 4.2

Let  $(a_1, c_1) \neq (a_2, c_2)$ . We will show that there exists  $(g_k)_{k \in \mathbb{N}} \subset L^2(S)$  with

$$|\langle (\Lambda_{a_1, c_1} - \Lambda_{a_2, c_2})g_k, g_k \rangle| \rightarrow \infty, \quad (10)$$

from which the assertion follows.

To this end, we apply the intuitive arguments explained in the beginning of section 4.1 in a rigorous manner. We start by noting that the measurements on  $S$  determine measurements on every open subset of  $S$ , so that w.l.o.g. we can assume that  $S$  is so small that there exists a connected neighborhood  $O$  of  $S$ , such that  $a_1, a_2, c_1$ , and  $c_2$  are constant, resp., analytic, on  $O$ .

We now distinguish the following three cases

- (a)  $a_1 \neq a_2$  on  $O$ ,
- (b)  $a_1 = a_2$ , but  $c_1 \neq c_2$  on  $O$ ,
- (c)  $a_1 = a_2$ , and  $c_1 = c_2$  on  $O$ .

Consider first case (a) and assume w.l.o.g. that  $a_2 > a_1$ . We apply theorem 3.1(a)(i) to obtain a sequence  $(g_k)_{k \in \mathbb{N}}$  such that the corresponding solutions  $(u_k)_{k \in \mathbb{N}}$  of (5) with coefficients  $(a_2, c_2)$  fulfill

$$\|u_k\|_{H^1(O)} \rightarrow \infty, \quad \|u_k\|_{L^2(O)} \rightarrow 0, \quad \text{and} \quad \|u_k\|_{H^1(B \setminus \bar{O})} \rightarrow 0.$$

Then it follows from lemma 4.1 that

$$\langle (\Lambda_{a_1, c_1} - \Lambda_{a_2, c_2})g_k, g_k \rangle \rightarrow \infty.$$

In case (b) we use an argument of Kohn and Vogelius [14]. There must be a smallest number  $l \in \mathbb{N}_0$  such that  $\partial_\nu^l(c_1 - c_2)|_S$  does not vanish everywhere on  $S$ , because otherwise all derivatives of  $c_2 - c_1$  would vanish on  $S$  which contradicts  $c_1 \neq c_2$ . (Note that we used here that  $c_1, c_2$  have an analytic extension to a neighborhood of  $\overline{O}$ .) Thus, there must be a connected neighborhood of an open subset of  $S$ , in which

$$c_1 \geq c_2, \quad \text{or} \quad c_1 \leq c_2. \quad (11)$$

W.l.o.g. we assume that  $S$  and  $O$  are already so small that (11) holds on the connected neighborhood  $O$  of  $S$ , and that  $c_2 \geq c_1$ . Also by analyticity,  $c_1 \neq c_2$  on  $O$ , so there exists an open subset  $O', \overline{O'} \subset O$  with  $(c_2 - c_1)|_{O'} \in L_+^\infty(O')$ . From theorem 3.1(a)(ii) we obtain a sequence  $(g_k)_{k \in \mathbb{N}}$  such that the corresponding solutions  $(u_k)_{k \in \mathbb{N}}$  of (5) with coefficients  $(a_2, c_2)$  fulfill

$$\|u_k\|_{L^2(O')} \rightarrow \infty, \quad \text{and} \quad \|u_k\|_{H^1(B \setminus \overline{O})} \rightarrow 0,$$

and again it follows from lemma 4.1 that

$$\langle (\Lambda_{a_1, c_1} - \Lambda_{a_2, c_2})g_k, g_k \rangle \rightarrow \infty.$$

Now we turn to case (c). We enlarge  $O$  to be a maximal connected component of the set where  $a_1 = a_2$  and  $c_1 = c_2$  that is a neighborhood of  $S$ . The boundary  $\partial O$  is a subset of the union of  $\partial B$  and the boundaries of the sets on which  $a_1, a_2, c_1$ , and  $c_2$  are piecewise constant, resp., analytic. Hence,  $\partial O$  is piecewise smooth. Also, there must be a smooth piece  $\Sigma$  of  $\partial O$  that does not intersect  $\partial B$  because otherwise  $\overline{O} \supset B$  and thus  $(a_1, c_1) = (a_2, c_2)$  on  $B$ . It follows that  $\Sigma$  lies in the interior of  $B$  and there exists a subset  $\Omega, \Omega \cap O = \emptyset$ , for which  $\Sigma \subset \partial \Omega$ . Possibly replacing  $\Sigma$  and  $\Omega$  by smaller sets we can assume that  $\Omega$  is connected,  $c_1, c_2$  are analytic on  $\Omega$  and  $a_1, a_2$  are constant on  $\Omega$ . From the maximality of  $O$ , we obtain that  $(a_1, c_1) \neq (a_2, c_2)$  on  $\Omega$ , so that one of the following two cases holds true.

(c1)  $a_1 \neq a_2$  on  $\Omega$ ,

(c2)  $a_1 = a_2$ , but  $c_1 \neq c_2$  on  $\Omega$ .

In the case of (c1) we assume again w.l.o.g. that  $a_2 > a_1$  and apply theorem 3.1(b)(i) to obtain  $(g_k)_{k \in \mathbb{N}}$  such that the corresponding solutions  $(u_k)_{k \in \mathbb{N}}$  of (5) with coefficients  $(a_2, c_2)$  fulfill

$$\|u_k\|_{H^1(\Omega)} \rightarrow \infty, \quad \|u_k\|_{L^2(\Omega)} \rightarrow 0, \quad \text{and} \quad \|u_k\|_{H^1(B \setminus \overline{O \cup \Omega})} \rightarrow 0.$$

Then, as above, lemma 4.1 yields (10) and thus the assertion.

In the finally remaining case of (c2) we obtain from the same arguments as above that, after possibly shrinking  $\Sigma$  and  $\Omega$  again, either

$$c_1 \geq c_2, \quad c_1 \neq c_2, \quad \text{or} \quad c_1 \leq c_2, \quad c_1 \neq c_2,$$

on  $\Omega$ . Assuming w.l.o.g. that the latter holds true, there exists an open subset  $\Omega'$ ,  $\overline{\Omega'} \subset \Omega$  with  $(c_2 - c_1)|_{\Omega'} \in L_+^\infty(\Omega')$ . We then apply theorem 3.1(b)(ii) to obtain  $(g_k)_{k \in \mathbb{N}}$  such that the corresponding solutions  $(u_k)_{k \in \mathbb{N}}$  of (5) with coefficients  $(a_2, c_2)$  fulfill

$$\|u_k\|_{L^2(\Omega')} \rightarrow \infty, \quad \text{and} \quad \|u_k\|_{H^1(B \setminus \overline{\Omega})} \rightarrow 0.$$

So, also in this last case, lemma 4.1 yields (10) and thus the assertion.  $\square$

## 5. Discussion and conclusions

The inherent non-uniqueness described in Arridge and Lionheart [3] makes it impossible to recover both an unknown diffusion and an unknown absorption distribution in dc diffuse optical tomography. Even the most idealized, complete and error-free measurements do not hold enough information for this task. Instead, there always exists an infinite number of combinations of diffusion and absorption profiles that is compatible with the measurements.

Every reconstruction algorithm (that uses the dc diffusion approximation) must choose one of these combinations and it can only do so by using additional information. This additional information may be implemented explicitly by a constraint (e.g. take the one which is piecewise constant), a preference (e.g. take the one with the smallest  $L^2$ -norm), or by possibly hidden constraints and preferences resulting from the implementation details (e.g. the discretization).

Given the arguments of [3] that smooth diffusion and absorption coefficients can be combined in one effective absorption parameter, cf (2), one may suspect that the needed additional information is essentially one of the two parameters, so that there is no hope in determining both coefficients. This interpretation is contradicted by successful simultaneous reconstructions of both parameters from phantom experiment data using the dc diffusion approximation model, cf e.g. Pei, Graber and Barbour [20] and Xu, Gu, Khan and Jiang [23].

Our result reconciles these seemingly contradictory theoretical and practical results. Though there is an infinite number of diffusion/absorption pairs leading to the same measurements, Theorem 4.2 shows that at most one of them consists of a piecewise constant diffusion and piecewise analytic absorption. If the true medium has these properties (as in the experimental works cited above) then a reconstruction algorithm favoring these properties will pick the right combination of profiles.

Hence, dc-measurements hold considerably more information about separately the diffusivity and the absorptivity of a domain than one would initially expect from the interchangeability of these coefficients. However, our assumptions (in particular the piecewise-constant diffusivity) may be too strong for many realistic cases. A precise characterization of the amount of information that dc measurements contain about more general coefficients still remains an important theoretical challenge.

In this work, a jump in the diffusivity could be distinguished from absorption effects, so that this may belong to the identifiable properties. Between the jumps we prevented

a cross-talk between diffusivity and absorptivity by assuming that the diffusivity  $a$  is constant, which in particular means that  $\Delta\sqrt{a} = 0$  in equation (2), which governs the interplay. This suggests another open question: Does uniqueness still hold true in the class of diffusivities that are piecewise smooth with harmonic square roots?

Finally, let us stress again that our result is derived in the context of an infinite-dimensional set of error-free measurements. In practice, one only has access to finitely many, noisy measurements, and reconstruction algorithms usually work with linearized, discrete settings. For electrical impedance tomography, Lechleiter and Rieder [17] have just derived convergence of a Newton-like regularization method from local injectivity results for a discrete setting. Using the localized potentials of theorem 3.1, one might be able to extend their results also to reconstruction algorithms in optical tomography.

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## Appendix

**Proof of lemma 4.1.** From the Lax-Milgram-Theorem (cf, e.g., Dautray and Lions [4, VII, §1, Rem. 3]) it follows that  $u_2$  minimizes the functional

$$w \mapsto \int_B (a_2 |\nabla w|^2 + c_2 |w|^2) \, dx - 2 \int_S g w|_S \, ds$$

in  $H^1(B)$ , so that

$$\begin{aligned} & - \int_B (a_2 |\nabla u_2|^2 + c_2 |u_2|^2) \, dx \\ &= \int_B (a_2 |\nabla u_2|^2 + c_2 |u_2|^2) \, dx - 2 \int_S g u_2|_S \, ds \\ &\leq \int_B (a_2 |\nabla u_1|^2 + c_2 |u_1|^2) \, dx - 2 \int_S g u_1|_S \, ds \\ &= \int_B (a_2 |\nabla u_1|^2 + c_2 |u_1|^2) \, dx - 2 \int_B (a_1 |\nabla u_1|^2 + c_1 |u_1|^2) \, dx, \end{aligned}$$

and thus

$$\begin{aligned} & \langle (\Lambda_{a_1, c_1} - \Lambda_{a_2, c_2})g, g \rangle \\ &= \int_B (a_1 |\nabla u_1|^2 + c_1 |u_1|^2) \, dx - \int_B (a_2 |\nabla u_2|^2 + c_2 |u_2|^2) \, dx \\ &\leq \int_B (a_1 |\nabla u_1|^2 + c_1 |u_1|^2) \, dx + \int_B (a_2 |\nabla u_1|^2 + c_2 |u_1|^2) \, dx \\ &\quad - 2 \int_B (a_1 |\nabla u_1|^2 + c_1 |u_1|^2) \, dx \end{aligned}$$

$$= \int_B ((a_2 - a_1)|\nabla u_1|^2 + (c_2 - c_1)|u_1|^2) dx.$$

This yields the first inequality in (8). The second one follows from interchanging  $(a_1, c_1)$  and  $(a_2, c_2)$ .  $\square$

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