SIAM J. MATH. ANAL.
Vol. 42, No. 5, pp. 1934–1948

ANALYSIS AND REGULARIZATION OF PROBLEMS IN DIFFUSE OPTICAL TOMOGRAPHY*

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Abstract. In this paper we consider the regularization of the inverse problem of diffuse optical tomography by standard regularization methods with quadratic penalty terms. We therefore investigate in detail the properties of the associated forward operators and derive continuity and differentiability results, which are based on derivation of $W^{1,p}$ regularity of solutions for the governing elliptic boundary value problems. We then show that Tikhonov regularization can be applied for a stable solution and that the standard convergence and convergence rates results hold. Our analysis also allows us to ensure convergence of iterative regularization methods, which are important from a practical point of view.

Key words. diffuse optical tomography, elliptic partial differential equations, regularity, parameter identification, inverse problems, regularization

AMS subject classifications. 35B65, 35R30, 49N45, 47A52, 78A46

DOI. 10.1137/090781590

1. Introduction.

Diffuse optical tomography is a noninvasive imaging technique that utilizes near-infrared light to probe highly scattering media. Typical applications include the monitoring of the oxygenation state of blood in the neonatal brains or the detection of breast cancer; see [3, 15, 22, 23].

The transport of light in highly scattering media is usually modeled by the diffusion approximation, which can be derived from moment expansions of the underlying, more basic radiative transfer equation [7, 3]. In case of continuous or intensity modulated excitation, this yields an elliptic boundary value problem describing mathematically the physics of light propagation in the sample of interest. The inverse problem of optical tomography then consists of determining the distribution of optical parameters from measurements of the transmitted light at the boundary. Uniqueness of solutions can be proved, if intensity modulated light is used for the excitation [24, 16, 21], but also nonuniqueness results are known, if one tries to simultaneously identify the distribution of absorption and diffusion coefficients using continuous wave excitation measurements [24, 4]. Since the mapping that associates optical parameters with measurements is compact (with respect to all reasonable topologies), the inverse problem is ill-posed. Therefore, some regularization method has to be used, in order to obtain stable solutions, in particular, in the presence of measurement perturbations.

In this paper, we investigate the applicability of Tikhonov regularization. While Tikhonov regularization provides a general framework for solving a large variety of linear and nonlinear inverse problems, also some other, problem adapted methods are available for optical tomography and similar applications. Let us mention the d-bar method [30, 6], which is motivated by analytical methods already used in uniqueness

*Received by the editors January 4, 2010; accepted for publication (in revised form) June 21, 2010; published electronically August 17, 2010. Financial support by the Austrian Science Fund (FWF) through grant SFB/F032 and by the German Science Foundation (DFG) via grant GSC 111 is gratefully acknowledged.

http://www.siam.org/journals/sima/42-5/78159.html

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proofs [29]; details of a numerical realization have been discussed in [34] for impedance tomography and in [2] for inverse scattering. A second class of methods is based on certain factorizations of the measurement operator. The resulting sampling methods are well established for electrical impedance tomography and acoustic scattering, but can also be applied to optical tomography [20, 14, 26]. Note that a connection between the factorization method and linear backprojection algorithms (or linearized Tikhonov regularization) can be established [10].

In order to apply standard regularization theory, we investigate in detail the properties of the nonlinear forward operator (the mapping of parameters to measurements). This forward operator has been considered previously in [9]; see also [31] for related results in impedance tomography. In these works, Banach space topologies (L^∞ or L^p, $p > 2$) are used in the parameter space, which simplifies the analysis of the forward operators considerably. In particular, using the L^∞-norm for the parameters, as in [9], continuity and Fréchet differentiability of the forward operator follow almost trivially. From a numerical point of view, it is, however, advantageous to utilize Hilbert space topologies for the parameter and measurement spaces, and we will adopt such an approach here. This not only facilitates the analysis of (the regularized solution of) the inverse problem but also simplifies the discretization and numerical solution of the resulting nonlinear (optimization) problems. The results of [9, 31] are not applicable to the setting investigated here; in fact, we require a much deeper analysis of the governing boundary value problems. Our results are based on certain $W^{1,p}$ a-priori estimates for solutions of the governing elliptic boundary value problem, which we establish under mild assumptions on the coefficients and the smoothness of the domain. Having developed such a detailed analysis of the forward operator, convergence results for nonlinear Tikhonov regularization can be derived with standard arguments.

The outline of the manuscript is as follows: After fixing the relevant notation, we introduce in section 2 the boundary value problem governing diffuse transport of light in tissue and define the forward operator, which maps optical parameters to virtual boundary measurements corresponding to one single excitation. In section 3, we investigate in detail the properties of this forward operator; i.e., we derive continuity and differentiability results, and show compactness and weak closedness, which are central properties for the regularization of the inverse problem. At the end of section 3, we also discuss the extension to multiple excitations. In section 4, we then formally introduce the inverse problem, we discuss its solution by Tikhonov regularization, and we summarize the basic convergence results, which are based on the results of section 3. A detailed derivation of regularity results for solutions to elliptic boundary value problems, which are required for our analysis, is given in the Appendix.

2. Basic notation and the physical model.

2.1. Basic notation and preliminaries. Throughout the text, $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, will denote a domain with (at least) Lipschitz regular boundary. For $1 \le p < \infty$, we denote by $L^p(\Omega)$ the standard Lebesgue space of power-p integrable (real or complex valued) functions with norm $\|f\|_{p;\Omega}^p = \int_\Omega |f(x)|^p dx$. The space $L^\infty(\Omega)$ of essentially bounded functions is equipped with the norm $\|u\|_{\infty;\Omega} = \operatorname{ess\,sup}_{x\in\Omega} |u(x)|$, and the scalar product $(u, v)_\Omega := \int_\Omega u\, \overline{v}\, dx$ is used for the Hilbert space $L^2(\Omega)$. By $W^{1,p}(\Omega)$, we denote the usual Sobolev space equipped with the norm $\|u\|_{1,p;\Omega}^p = \|u\|_{p;\Omega}^p + \|\nabla u\|_{p;\Omega}^p$. The space $H^1(\Omega) := W^{1,2}(\Omega)$ with scalar product $(u, v)_{1,\Omega} :=$

$(u, v)_\Omega + (\nabla u, \nabla v)_\Omega$ is again a Hilbert space. Spaces, norms, and scalar products for functions defined on the boundary $\partial\Omega$ are defined accordingly.

We will frequently make use of the following embedding theorems; for proofs and general material on Sobolev spaces, we refer to the book by Adams [1].

THEOREM 2.1 (embedding theorems). (a) *The embedding* $W^{1,p}(\Omega) \to L^q(\Omega)$ *is continuous if* (i) $d > p$ *and* $q \le dp/(d-p) =: p^*$ *or* (ii) $d \le p$ *and* $1 < q < \infty$. *For* (i) *with* $q < p^*$ *or* (ii), *the embeddings are compact.*

(b) *The embedding (trace map)* $W^{1,p}(\Omega) \to L^r(\partial\Omega)$ *is continuous if* (i) $d > p$ *and* $r \le (d-1)p/(d-p) =: p^\circ$ *or* (ii) $d \le p$ *and* $1 < r < \infty$. *Again, for* (i) *with* $r < p^\circ$ *or* (ii), *the embedding is compact.*

Throughout the text, C will denote a generic constant, whose value may depend on the context.

2.2. Physical model and basic assumptions. The propagation of intensity modulated light in highly scattering media can be described by the diffusion approximation [3]

$$-\mathrm{div}(\kappa \nabla \Phi) + (\mu + ik)\Phi = 0 \qquad \text{in } \Omega, \tag{1}$$

where Φ is the complex amplitude of the photon density, μ is the absorption rate per unit length, and $k = \omega/c$ is the wave number with ω the modulation frequency and c the speed of light. The photon diffusion coefficient is given by $\kappa = 1/(d\ (\mu + \mu_s'))$, where μ_s' is the reduced scattering rate per unit length, and d is the spatial dimension. The system is completed with Robin boundary conditions [28]

$$\kappa \partial_n \Phi = \rho\,(q - \Phi) \qquad \text{on } \partial\Omega, \tag{2}$$

which model a diffuse light source located at the boundary. The positive parameter function ρ allows us to take into account a refractive index mismatch between Ω and the surrounding space [18]. We will write Φ_q if the dependence of the solution on the source q shall be emphasized.

In order to ensure solvability of the boundary value problem (1)–(2), we impose the following basic conditions on the coefficients.

Assumption 2.2.

(i) The function ρ is uniformly positive and bounded; i.e., there exist positive constants $\underline{\rho}$, $\overline{\rho}$ such that $\underline{\rho} \le \rho \le \overline{\rho}$ on $\partial\Omega$.

(ii) The function κ is uniformly positive and bounded; i.e., there exist $\underline{\kappa}$, $\overline{\kappa} > 0$ such that $\underline{\kappa} \le \kappa \le \overline{\kappa}$ on Ω.

(iii) The function $\mu \in L^\infty(\Omega)$ is non-negative and bounded from above; i.e., there exists $\overline{\mu}$ such that $0 \le \mu \le \overline{\mu}$.

The following result is a special case of Theorem A1, which is based on the complex version of the Lax–Milgram theorem.

THEOREM 2.3. *Let Assumption* 2.2 *hold. Then, for any source* $q \in L^2(\partial\Omega)$, *the boundary value problem* (1)–(2) *have a unique (complex valued) solution* $\Phi \in H^1(\Omega)$ *that satisfies*

$$\|\Phi\|_{1,2;\Omega} \le C \|q\|_{2;\partial\Omega} \tag{3}$$

with a constant C *depending only on the domain* Ω *and the bounds of the coefficients in Assumption* 2.2.

2.3. Measurements. The measurable quantity in optical tomography is the complex amplitude of the photon flux leaving the domain Ω, i.e., $-\kappa\partial_n\Phi$, which by (2) equals $\rho\,(\Phi - q)$. We define the observation operator

$$B\colon H^1(\Omega) \to L^2(\partial\Omega), \qquad \Phi \mapsto \rho\,(\Phi - q)|_{\partial\Omega}, \tag{4}$$

which associates with a function $\Phi \in H^1(\Omega)$ its trace $\rho(\Phi - q)$ at the boundary. The following result is a direct consequence of Theorem 2.1.

LEMMA 2.4. *Let $q \in L^2(\partial\Omega)$ be given and Assumption 2.2 hold. Then the observation operator $B\colon H^1(\Omega) \to L^2(\partial\Omega)$ is a bounded, compact, affine linear operator.*

We will write B_q instead of B, if we want to emphasize the dependence of B on the source q.

Remark 2.5. In practice, the light intensities at the boundary are measured by finitely many detectors d_i, $i = 1, \dots, nd$, e.g., a digital camera. This case can be considered similarly, by modifying the definition of the observation operator accordingly. Since nd will typically be large, we consider the limit case of continuous observation in what follows and come back to the case of finite observations in section 3.4.

2.4. Forward operator. In an optical experiment, an object is illuminated by a light source q, and the resulting light intensity $B(\Phi)$ is measured at the boundary. This establishes a nonlinear relation between the optical parameters κ and μ characterizing the medium and the corresponding measurements $B(\Phi)$. A mathematical model of such an experiment for a single source q is the following.

DEFINITION 2.6 (forward operator). *For given source $q \in L^2(\partial\Omega)$, define*

$$F\colon \mathcal{D}(F) \to L^2(\partial\Omega), \qquad (\kappa, \mu) \mapsto B(\Phi), \tag{5}$$

where Φ denotes the solution of the elliptic boundary value problem (1)–(2).

We will use the notation F_q, if the dependence of the operator F on the source q has to be emphasized. Because of Theorem 2.3 and Lemma 2.4, the forward operator is well defined for parameters in the admissible set

$$\mathcal{D}(F) = \{(\kappa, \mu) \in L^2(\Omega) \times L^2(\Omega)\colon \text{ Assumption 2.2 is satisfied}\}. \tag{6}$$

Remark 2.7. In the following, we consider in detail the forward operator for a single source q. The extension to the practically relevant case of finitely many excitations q_j, $j = 1, \dots, ns$ or to infinitely many excitations is discussed in section 3.4.

3. Properties of the forward operator.

In this section, we investigate in detail the mapping properties of the forward operator F; i.e., we prove results concerning continuity and compactness, and we derive certain differentiability properties.

3.1. Continuity and compactness of the forward operator. Throughout, we assume that the forward operator $F\colon \mathcal{D}(F) \to L^2(\partial\Omega)$ is defined according to (5) for some given source term $q \in L^2(\partial\Omega)$. If not stated otherwise, the preimage and image spaces of the operator F are equipped with the topologies of $H^1(\Omega) \times L^2(\Omega)$ and $L^2(\partial\Omega)$, respectively. Some of our results, however, hold with respect to a weaker topology in the parameter space, and we comment on this in remarks.

Remark 3.1. The set of admissible parameters $\mathcal{D}(F)$ is closed and convex, but it has no interior points; i.e., for any $(\kappa, \mu) \in \mathcal{D}(F)$ the ball $\mathcal{B}_\epsilon(\kappa, \mu) := \{(\tilde\kappa, \tilde\mu) \in \mathcal{D}(F)\colon \|\kappa - \tilde\kappa\|^2_{1,2;\Omega} + \|\mu - \tilde\mu\|^2_{2;\Omega} < \epsilon^2\}$ is not completely contained in $\mathcal{D}(F)$ for any $\epsilon > 0$. Therefore, all results stated below have to be understood with respect to the relative topology.

THEOREM 3.2 (continuity). *The operator $F\colon \mathcal{D}(F) \to L^2(\partial\Omega)$ is continuous.*

Proof. Let $\{(\kappa_n, \mu_n)\} \subset \mathcal{D}(F)$ be a sequence converging to (κ, μ) in $H^1(\Omega) \times L^2(\Omega)$. Since the set $\mathcal{D}(F)$ is closed, the limit $(\kappa, \mu) \in \mathcal{D}(F)$. Now let Φ_n and Φ denote the (weak) solutions of the boundary value problem (1)–(2) with parameters (κ_n, μ_n) and (κ, μ), respectively. Since by Theorem 2.3, the solutions Φ_n are uniformly bounded in $H^1(\Omega)$, there exists a weakly convergent subsequence (again denoted by Φ_n) such that $\Phi_n \rightharpoonup y$ weakly in $H^1(\Omega)$ for some $y \in \mathcal{D}(F)$. By linearity of (1) and (2), the difference $w_n := \Phi_n - \Phi$ satisfies

$$
\begin{aligned}
(7) \qquad &(\kappa \nabla w_n, \nabla v)_\Omega + ((\mu + ik) w_n, v)_\Omega + (\rho w_n, v)_{\partial\Omega} \\
&\qquad = ((\kappa_n - \kappa)\nabla \Phi_n, \nabla v)_\Omega + ((\mu_n - \mu)\Phi_n, v)_\Omega =: (*)
\end{aligned}
$$

for every $v \in C^\infty(\overline{\Omega})$. Using the Cauchy–Schwarz and Hölder inequalities, we obtain

$$
\big|(*)\big| \le \|\kappa_n - \kappa\|_{2;\Omega} \|\nabla \Phi_n\|_{2;\Omega} \|\nabla v\|_{\infty;\Omega} + \|\mu_n - \mu\|_{2;\Omega} \|\Phi_n\|_{2;\Omega} \|v\|_{\infty;\Omega}.
$$

Thus, convergence of $\kappa_n \to \kappa$ in $H^1(\Omega)$ and $\mu_n \to \mu$ in $L^2(\Omega)$ imply convergence of the right-hand side of (7) to zero. The weak limit $w = y - \Phi$ then is a solution of the variational problem

$$
(\kappa \nabla w, \nabla v)_\Omega + ((\mu + ik) w, v)_\Omega + (w, v)_\Omega = 0,
$$

and by density of $C^\infty(\overline{\Omega})$ in $H^1(\Omega)$ and Theorem 2.3, we obtain $w \equiv 0$. This shows that $\Phi_n \rightharpoonup \Phi$ weakly in $H^1(\Omega)$, and by the definition of F and the compactness of the observation operator B, we obtain that $F(\kappa_n, \mu_n) \to F(\kappa, \mu)$ strongly in $L^2(\partial\Omega)$ (for this subsequence). The result now follows by observing that the same arguments hold for any subsequence of $\{\Phi_n\}$, and every limit satisfies the same variational problem, which has a unique solution. $\square$

Remark 3.3. A careful inspection of the previous proof shows that F is continuous also with respect to the weaker topology of $L^2(\Omega) \times L^2(\Omega)$ for the parameter space.

COROLLARY 3.4 (compactness). *The operator $F\colon \mathcal{D}(F) \to L^2(\partial\Omega)$ is compact.*

Proof. It follows from the proof of Theorem 3.2 that the mapping $(\kappa, \mu) \mapsto \Phi$ is continuous with respect to the $H^1(\Omega) \times L^2(\Omega)$ and $H^1(\Omega)$ topologies. Moreover, by Lemma 2.4, the mapping $\Phi \mapsto B(\Phi)$ is compact (as mapping from $H^1(\Omega)$ to $L^2(\partial\Omega)$). Hence F is compact, since it is the concatenation of a continuous and a compact mapping. $\square$

As we will show below, the inverse problem of optical tomography is ill-posed due to the compactness of the forward operator F. In order to apply standard results of regularization theory, we will require the following basic property.

THEOREM 3.5 (weak closedness). *The operator $F\colon \mathcal{D}(F) \to L^2(\partial\Omega)$ is (sequentially) closed with respect to the weak topologies of $H^1(\Omega) \times L^2(\Omega)$ and $L^2(\partial\Omega)$; i.e., if $(\kappa_n, \mu_n) \rightharpoonup (\kappa, \mu)$ weakly in $H^1(\Omega) \times L^2(\Omega)$, then $(\kappa, \mu) \in \mathcal{D}(F)$ and $F(\kappa_n, \mu_n) \rightharpoonup F(\kappa, \mu)$ weakly in $L^2(\partial\Omega)$.*

Proof. Since $\mathcal{D}(F)$ is closed and convex, it is weakly closed [32, Thm. 3.12], and consequently the weak limit $(\kappa, \mu) \in \mathcal{D}(F)$. Because of the compact embedding of $H^1(\Omega) \hookrightarrow L^2(\Omega)$, we have $\kappa_n \to \kappa$ (strongly) in $L^2(\Omega)$. Moreover, using the notation of the proof of Theorem 3.2, we obtain that $\Phi_n \to \Phi$ in $L^2(\Omega)$ and thus $((\mu_n - \mu)\Phi_n, v)_\Omega \to 0$ (see (7)). It then follows from Remark 3.3 that $F(\kappa_n, \mu_n) \to F(\kappa, \mu)$ strongly in $L^2(\partial\Omega)$. $\square$

As the proof of the previous theorem reveals, the operator F actually maps weakly converging sequences to strongly convergent sequences.

COROLLARY 3.6. *The operator* $F\colon \mathcal{D}(F) \to L^2(\partial\Omega)$ *is completely continuous; i.e., if* $(\kappa_n, \mu_n) \rightharpoonup (\kappa, \mu)$ *weakly in* $H^1(\Omega) \times L^2(\Omega)$*, then* $F(\kappa_n, \mu_n) \to F(\kappa, \mu)$ *strongly in* $L^2(\partial\Omega)$.

Remark 3.7. The two previous results essentially rely on the compact embedding of $H^1(\Omega) \hookrightarrow L^2(\Omega)$, which is used to obtain strong convergence of $\kappa_n \to \kappa$ in $L^2(\Omega)$. In fact, the results derived so far remain valid, if other spaces that are compactly embedded in $L^2(\Omega)$ are used for defining an appropriate weak topology in the parameter space.

3.2. Hölder and Lipschitz continuity. In the following, we derive Hölder and Lipschitz continuity results for the forward operator. For proving these properties, we require some additional regularity of solutions to the governing boundary value problem (1)–(2). The basis for our results is a theorem due to Meyers [27], which states that the (weak) solution of the problem

$$\operatorname{div}(\kappa\nabla u) = \operatorname{div}(f) + g \qquad \text{in } \Omega,$$

lies in $W^{1,p}(\Omega)$ whenever $f \in L^p(\Omega, \mathbb{R}^d)$ and $g \in L^q(\Omega)$, $q' = (p')^\circ$ for some $p > 2$ depending on the domain Ω and the bounds for the parameter κ. The following result, which is proven in detail in the Appendix, can then be derived by perturbation arguments. For ease of notation, let us define for $1 < p < \infty$ the dual index $p' := \frac{p}{p-1}$, and $\bar{p} := ((p')^*)'$, $\hat{p} := ((p')^\circ)'$, where p^* and p° are as in Theorem 2.1.

THEOREM 3.8. *Let Assumption* 2.2 *hold. Then there exists a constant* $p_0 > 2$ *depending only on the domain and the bounds for the coefficients, such that the solution* u *of the variational problem*

$$(8) \qquad \begin{aligned} &(\kappa\nabla u, \nabla v)_\Omega + ((\mu + ik)u, v)_\Omega + (\rho u, v)_{\partial\Omega} \\ &\qquad = (f, \nabla v)_\Omega + (g, v)_\Omega + (\rho q, v)_{\partial\Omega} \qquad \textit{for all } v \in C^\infty(\overline{\Omega}) \end{aligned}$$

lies in $W^{1,p}(\Omega)$ *whenever* $f \in L^p(\Omega, \mathbb{R}^d)$, $g \in L^{\bar{p}}(\Omega)$, *and* $q \in L^{\hat{p}}(\partial\Omega)$ *for some* $p_0' \le p \le p_0$. *Moreover, there holds the a-priori estimate*

$$\|u\|_{1,p;\Omega} \le C\big(\|f\|_{p;\Omega} + \|g\|_{\bar{p};\Omega} + \|q\|_{\hat{p};\partial\Omega}\big)$$

with a constant C *that depends only on* Ω *and the bounds for the coefficients. If the domain* Ω *has a smooth boundary, and if* $\overline{\kappa}/\underline{\kappa}$ *approaches one, then the maximal* p_0*, such that the statement of the theorem holds, tends to infinity.*

Remark 3.9. The indices $\bar{p}$ and $\hat{p}$ arise from Hölder's inequality and embedding theorems. For dimension $d = 2$ and $p > 2$ we have $\bar{p} = 2p/(2 + p)$ and $\hat{p} = p/2$. Similarly, for $d = 3$ and $p > 3/2$ there holds $\bar{p} = 3p/(3 + p)$ and $\hat{p} = 2p/3$. If $d = 2$ and $p \le 2$, or $d = 3$ and $p \le 3/2$, then $\bar{p}$ and $\hat{p}$ can be chosen to be any number in $(1, \infty)$.

As a first consequence of this theorem, we obtain a uniform regularity result for solutions of the forward problem (1)–(2).

COROLLARY 3.10. *Let Assumption* 2.2 *hold, and let* Φ *denote the solution of* (1) *and* (2) *for some* $q \in L^2(\partial\Omega)$. *Then* $\Phi \in W^{1,p}(\Omega)$ *for some* $p > 2$*, and there holds the uniform bound* $\|\Phi\|_{1,p;\Omega} \le C\|q\|_{2;\partial\Omega}$ *with a constant* C *depending only on the domain and the bounds for the coefficients. If* Ω *is smooth and* $\overline{\kappa}/\underline{\kappa}$ *is sufficiently close to one, then the estimate holds, in particular, for every* $3/2 \le p \le 3$.

Proof. The assumption $q \in L^2(\partial\Omega)$ implies the condition $\hat{p} \le 2$, which in view of Remark 3.9 yields the restriction $p \le 3$ for $d = 2, 3$ space dimensions; the lower bound arises from duality arguments. The result then follows from Theorem 3.8 and Remark 3.9. Note that the bounds on p could be relaxed, if q is assumed to be more regular. ∎

Using this a-priori result on regularity of solutions Φ, we can specify the continuous dependence of the solution Φ on the parameters κ and μ more precisely.

THEOREM 3.11. *Let Assumption* 2.2 *hold, and let* Φ *and* $\tilde{\Phi}$ *denote the solutions of problem* (1)–(2) *with* $q \in L^2(\partial\Omega)$ *for parameters* (κ,μ) *and* $(\tilde{\kappa},\tilde{\mu})$*, respectively. Then*

$$\|\tilde{\Phi} - \Phi\|_{1,2;\Omega} \le C\big(\|\tilde{\kappa} - \kappa\|_{1,2;\Omega}^{\eta} + \|\tilde{\mu} - \mu\|_{2;\Omega}\big)\|q\|_{2;\partial\Omega},$$

with a constant C *depending only on the bounds of the parameters and the domain. The Hölder index is given by* $\eta = \min\{(3p-6)/p, 1\}$ *with* p *from Corollary* 3.10.

Proof. Let us define $\delta\kappa := \tilde{\kappa} - \kappa$ and $\delta\mu := \tilde{\mu} - \mu$. Then $w := \tilde{\Phi} - \Phi$ satisfies

$$(\kappa\nabla w, \nabla v)_\Omega + ((\mu + ik)w, v)_\Omega + (\rho w, v)_{\partial\Omega} = -(\delta\kappa\nabla\tilde{\Phi}, \nabla v)_\Omega - (\delta\mu\, \tilde{\Phi}, v)_\Omega$$

for all $v \in H^1(\Omega)$. By continuous embedding of $H^1(\Omega) \hookrightarrow L^6(\Omega)$ (in $d = 2, 3$ space dimensions) and noting that $\|\tilde{\Phi}\|_{1,p;\Omega} \le C\|q\|_{2;\partial\Omega}$ for some $p > 2$ by Corollary 3.10, we obtain by Hölder's inequality

$$\|\delta\kappa\nabla\tilde{\Phi}\|_{2;\Omega} \le \|\delta\kappa\|_{2p/(p-2);\Omega}\|\tilde{\Phi}\|_{1,p;\Omega}, \qquad \|\delta\mu\, \tilde{\Phi}\|_{5/6;\Omega} \le \|\delta\mu\|_{2;\Omega}\|\tilde{\Phi}\|_{1,2;\Omega}.$$

If $p = 3$, then $\|\delta\kappa\|_{2p/(p-2);\Omega} \le \|\delta\kappa\|_{6;\Omega} \le C\|\delta\kappa\|_{1,2;\Omega}$, and the results follow with $\eta = 1$. For $2 \le p \le 3$, we obtain by interpolation

$$\|\delta\kappa\|_{2p/(p-2);\Omega} \le C'\overline{\kappa}^{\frac{6-2p}{p}}\|\delta\kappa\|_{6;\Omega}^{\frac{3p-6}{p}} \le C\|\delta\kappa\|_{1,2;\Omega}^{\frac{3p-6}{p}},$$

which yields the result with $\eta = 3(p-2)/p$. Note that for $p \to 3$ the index η tends to one, and $\eta \to 0$ for p tending to 2. ∎

COROLLARY 3.12 (Hölder continuity). *Let the assumptions of Theorem* 3.11 *hold. Then the forward operator* $F{:}\mathcal{D}(F) \to L^2(\partial\Omega)$ *is Hölder continuous with respect to the topologies of* $H^1(\Omega) \times L^2(\Omega)$ *and* $L^2(\partial\Omega)$.

COROLLARY 3.13 (Lipschitz continuity). *Let the assumptions of Theorem* 3.11 *hold. If* $d = 2$*, or if* $d = 3$ *and additionally* Ω *is smooth and* $\overline{\kappa}/\underline{\kappa}$ *is sufficiently close to one, then* F *is Lipschitz continuous with respect to the topologies of* $H^1(\Omega) \times L^2(\Omega)$ *and* $L^2(\partial\Omega)$.

Proof. For space dimension $d = 2$, we have $H^1(\Omega) \hookrightarrow L^r(\Omega)$ for all $1 < r < \infty$, which allows us to estimate $\|\delta\kappa\|_{2p/(p-2);\Omega} \le C\|\delta\kappa\|_{1,2;\Omega}$, and the result follows along the lines of the proof of Theorem 3.11. The Lipschitz continuity for $d = 3$ follows directly from Theorem 3.11, and the mapping properties of the observation operator B. ∎

3.3. Results on differentiability. The Lipschitz continuity of the forward operator F indicates that a certain differentiability might be expected. Since differentiability is a key property for the convergence of iterative algorithms for the solution of nonlinear operator equations, as well as for the derivation of quantitative estimates in regularization theory, we will derive some results in this direction. For the following considerations, we assume that $d = 2$, or that $d = 3$ and additionally Ω is smooth and $\overline{\kappa}/\underline{\kappa}$ is sufficiently close to one, such that the forward operator is Lipschitz continuous, cf. Corollary 3.13.

THEOREM 3.14 (differentiability). *Let* $q \in L^2(\partial\Omega)$ *be given, and let* $(\kappa,\mu) \in \mathcal{D}(F)$ *and* $(\delta\kappa,\delta\mu) \in H^1(\Omega) \times L^2(\Omega)$ *such that* $(\kappa + t\delta\kappa, \mu + t\delta\mu) \in \mathcal{D}(F)$ *for all* $t \in \mathbb{R}$ *with*

$|t|$ sufficiently small. Then the derivative of F at (κ,μ) in direction $(\delta\kappa,\delta\mu)$ is given by $F'(\kappa,\mu)[\delta\kappa,\delta\mu]=\rho w|_{\partial\Omega}$, where w solves the sensitivity problem

$$(\kappa\nabla w,\nabla v)_\Omega+((\mu+ik)w,v)_\Omega+(\rho w,v)_{\partial\Omega}=-(\delta\kappa\nabla\Phi,\nabla v)_\Omega-(\delta\mu\Phi,v)_\Omega \tag{9}$$

for all $v\in H^1(\Omega)$, and Φ denotes the solution of problem (1)–(2). *Moreover, there holds the uniform estimate*

$$\|F'(\kappa,\mu)[\delta\kappa,\delta\mu]\|_{2;\partial\Omega}\le C\big(\|\delta\kappa\|_{1,2;\Omega}+\|\delta\mu\|_{2;\Omega}\big)\|q\|_{2;\partial\Omega} \tag{10}$$

with a constant C depending only on Ω and the bounds of the coefficients.

Proof. The result follows similarly to Theorem 3.11 and Corollary 3.13. □

THEOREM 3.15. *Let the assumptions of Theorem* 3.14 *hold. Then $F'(\kappa,\mu)[\delta\kappa,\delta\mu]$ defines a bounded linear operator $F'(\kappa,\mu){:}H^1(\Omega)\times L^2(\Omega)\to L^2(\partial\Omega)$, and the estimate* (10) *holds for all $(\delta\kappa,\delta\mu)\in H^1(\Omega)\times L^2(\Omega)$.*

Proof. The set $\mathcal{B}_\epsilon(\kappa,\mu)\cap\mathcal{D}(F)$ is dense in $\mathcal{B}_\epsilon(\kappa,\mu):=\{(\tilde\kappa,\tilde\mu){:}\|\tilde\kappa-\kappa\|^2_{H^1(\Omega)}+\|\tilde\mu-\mu\|^2_{L^2(\Omega)}\le\epsilon^2\}$, and thus $F'(\kappa,\mu)$ is densely defined by the directional derivatives, and uniformly bounded by (10). By the uniform boundedness principle there exists a unique continuous extension, again denoted by $F'(\kappa,\mu)$. □

For the proof of convergence rates or the convergence of iterative regularization methods, we will utilize that the derivative operator is Lipschitz continuous, which is a direct consequence of the following estimate.

THEOREM 3.16. *Assume that Ω is smooth and that either $d=2$ or $d=3$ and $\overline{\kappa}/\underline{\kappa}$ is sufficiently close to one such that Theorem* 3.8 *holds with $p_0=3$. Then the linear Taylor expansion of F around $(\kappa,\mu)\in\mathcal{D}(F)$ is second order accurate; i.e., for $(\tilde\kappa,\tilde\mu)\in\mathcal{D}(F)$ there holds*

$$\begin{aligned}\|F(\tilde\kappa,\tilde\mu)-F(\kappa,\mu)-F'(\kappa,\mu)[\tilde\kappa-\kappa,\tilde\mu-\mu]\|_{2;\partial\Omega}&\\ \le C_L\Big(\|\tilde\kappa-\kappa\|^2_{1,2;\Omega}+\|\tilde\mu-\mu\|^2_{2;\Omega}\Big)\|q\|_{2;\partial\Omega},&\end{aligned}$$

with a constant C_L depending only on the domain Ω and the bounds for the coefficients in Assumption 2.2.

Proof. Let Φ and $\tilde\Phi$ denote the solution of the forward problem (1)–(2) with parameters $(\tilde\kappa,\tilde\mu)$ and (κ,μ), respectively. Moreover, let w be the solution of (9), and define $\delta\kappa:=\tilde\kappa-\kappa$ and $\delta\mu:=\tilde\mu-\mu$. Then the function $z:=\tilde\Phi-\Phi-w$ satisfies the variational problem

$$\begin{aligned}(\kappa\nabla z,\nabla v)_\Omega+((\mu+ik)z,v)_\Omega+(\rho z,v)_{\partial\Omega}&\\ =-(\delta\kappa\nabla(\tilde\Phi-\Phi),\nabla v)_\Omega-(\delta\mu\,(\tilde\Phi-\Phi),v)_\Omega&\end{aligned}$$

for all $v\in H^1(\Omega)$. Application of Hölder's inequality yields

$$\|\delta\kappa\nabla(\tilde\Phi-\Phi)\|_{3/2;\Omega}\le\|\delta\kappa\|_{6;\Omega}\|\tilde\Phi-\Phi\|_{1,2;\Omega}.$$

Thus, by Theorem 3.8 with $p=3/2$, the solution of this variational problem satisfies $z\in W^{1,3/2}(\Omega)$, and the result follows by Corollary 3.13, by the continuous embedding of $H^1(\Omega)\hookrightarrow L^6(\Omega)$, and by the continuity of the trace mapping $W^{1,3/2}(\Omega)\to L^2(\partial\Omega)$ in $d=2,3$ dimensions. □

A careful inspection of the previous proof reveals that the H^1 topology provides the minimal regularity for the parameter κ in order to obtain the Lipschitz continuity of the derivative. This is an important property for the analysis of the inverse problem presented in the next section.

3.4. Finitely many measurements and multiple excitations. At the end of this section, let us discuss some generalizations of the results derived in this section.

Remark 3.17 (finite observations). In practice, the light intensities at the boundary are measured at finitely many locations, e.g., by a digital camera. One pixel then integrates the photon flux over some area Γ_i, and the corresponding observation operator is given by

$$B^{nd} : H^1(\Omega) \to \mathbb{C}^{nd}, \qquad \Phi \mapsto \left[\frac{1}{|\Gamma_i|}\int_{\Gamma_i} \rho(\Phi - q)\, ds\right]_{1\le i\le nd}.$$

Note that B^{nd} can be obtained from B by projection to a finite dimensional space; i.e., $B^{nd} = DB$ where $D{:}L^2(\partial\Omega) \to \mathbb{C}^{nd}$ is a bounded linear operator. This follows from the Cauchy–Schwarz inequality

$$\int_{\Gamma_i} \rho(\Phi - q)\, ds \le C|\Gamma_i|^{1/2}\|\Phi - q\|_{2;\Gamma_i}.$$

Hence by Lemma 2.4, B^{nd} is a continuous (compact) operator from $H^1(\Omega) \to \mathbb{C}^{nd}$, and all properties derived for the forward operator F with continuous measurements also hold for the operator $F^{nd} := D \circ F$ with finite measurement setup.

As a second extension of our results, let us consider the practically relevant case of finitely many excitations q_j, $j = 1, \dots, ns$. The analysis of this case can be reduced to the case of a single excitation as follows.

Remark 3.18 (multiple excitations). Let us define the forward operator

$$F\colon \mathcal{D}(F) \to [L^2(\partial\Omega)]^{ns}, \qquad (\kappa, \mu) \mapsto [F_{q_1}(\kappa, \mu), \dots, F_{q_{ns}}(\kappa, \mu)],$$

which maps the optical parameters to the collection of measurements corresponding to multiple sources q_j, $j = 1, \dots, ns$. Here F_{q_j} denotes the forward operator for single source q_j as defined above. All properties stated for the operator $F = F_q$ for a single source carry over verbatim to the case of finitely many excitations.

From a mathematical point of view, it is also interesting to study the idealized setting of infinitely many sources.

Remark 3.19 (idealized forward operator). The set of measurements for all possible sources $q \in L^2(\partial\Omega)$ defines a bounded linear operator

$$\mathcal{M}\colon L^2(\partial\Omega) \to L^2(\partial\Omega), \qquad q \mapsto \mathcal{M}q := B_q(\Phi_q),$$

which associates with each source q the corresponding measurement of the light intensity Φ_q defined by (1) and (2). Since $B_q(\Phi_q) = \rho(\Phi_q - q) = -\partial_n \Phi_q$, the output $\mathcal{M}$ is just the *Robin-to-Neumann* map of the boundary value problem (1)–(2). Let us define the *idealized forward operator*

$$\mathcal{F}\colon D(F) \to \mathcal{L}(L^2(\partial\Omega), L^2(\partial\Omega)), \qquad (\kappa, \mu) \mapsto \mathcal{M}.$$

If $\partial\Omega$ is sufficiently smooth, and $\overline{\kappa}/\underline{\kappa}$ is sufficiently close to one, then all properties of the forward operator F (for a single source) derived in this section also hold for the idealized operator $\mathcal{F}$. To see this, note that the statements and proofs of Theorems 3.11, 3.14, 3.15, 3.16 and Corollaries 3.12, 3.13 hold uniformly with respect to q. The corresponding statements for the idealized forward operator $\mathcal{F}$ then are obtained from the properties of F by using the definition of the norm of $\mathcal{L}(L^2(\partial\Omega), L^2(\partial\Omega))$, i.e.,

$$\|\mathcal{M}\|_{\mathcal{L}(L^2(\partial\Omega, L^2(\partial\Omega)))} = \sup_{q\neq 0} \frac{\|\mathcal{M}q\|_{L^2(\partial\Omega)}}{\|q\|_{L^2(\partial\Omega)}},$$

and the uniform bounds of the estimates with respect to q. In this way, the results obtained for a single source can be lifted to the case of infinitely many sources.

4. Inverse problem. The inverse problem of diffuse optical tomography is to find the parameters $(\kappa, \mu) \in \mathcal{D}(F)$ which correspond to the data y^δ. Mathematically, this means to solve the nonlinear operator equation

$$F(\kappa, \mu) = y^\delta, \quad (\kappa, \mu) \in \mathcal{D}(F), \quad y^\delta \in L^2(\partial\Omega). \tag{11}$$

Here, y^δ denotes the (possibly perturbed) measurement of the true data y, for which the inverse problem is assumed to have a solution for physical reasons; i.e., there exists (κ, μ) such that $F(\kappa, \mu) = y$. Because of the compactness of the forward operator F (cf. Corollary 3.4), the inverse problem (11) is ill-posed, and thus some regularization method has to be used in order to obtain a stable solution. In the following, we consider Tikhonov regularization; i.e., we define an approximate solution $(\kappa_\alpha^\delta, \mu_\alpha^\delta)$ as a minimizer of the Tikhonov functional

$$J_\alpha(\kappa, \mu) := \frac{1}{2}\|F(\kappa, \mu) - y^\delta\|^2 + \frac{\alpha}{2}\left(\|\kappa - \kappa_0\|_{1,2;\Omega}^2 + \|\mu - \mu_0\|_{2;\Omega}^2\right) \tag{12}$$

in $\mathcal{D}(F)$. The element (κ_0, μ_0) serves as an a-priori guess for the unknown parameters, and a positive regularization parameter $\alpha > 0$ allows us to establish the existence of minimizers and stability of the solution process.

Remark 4.1. The operator F used in the definition of the Tikhonov functional can be either of the forward operators discussed in section 3.4. If F denotes the forward operator for a single source and continuous measurements, then the norm for the least squares term is defined as $\|F(\kappa, \mu) - y^\delta\| := \|F(\kappa, \mu) - y^\delta\|_{0;\partial\Omega}$. To consider the case of finitely many excitations, one would define $\|F(\kappa, \mu) - y^\delta\|^2 := \frac{1}{ns}\sum_{j=1}^{ns} \|F_{q_j}(\kappa, \mu) - y_j^\delta\|_{0;\partial\Omega}^2$ instead. An appropriate norm for discrete observations and finitely many sources would be given by $\|F^{nd}(\kappa, \mu) - y^\delta\|^2 := \frac{1}{ns\cdot nd}\sum_{i=1}^{nd}\sum_{j=1}^{ns} |B_{i,q_j}^{nd}(\Phi_{q_j}) - y_{ij}^\delta|^2$. Since all three forward operators share the same properties, the following results concerning the regularized solution of the inverse problem hold for all three cases. We therefore use a generic norm $\|\cdot\|$ in the definition of the Tikhonov functional.

Remark 4.2 (uniqueness). One can show that under additional assumptions on the parameters, the inverse problem of diffuse optical tomography has a unique solution, if measurements are taken for infinitely many excitations, i.e., if the full Robin-to-Neumann map is measured. For results in this direction, see [4, 16, 21]. In case of one single or finitely many excitations, uniqueness cannot be expected. One then searches for a (κ_0, μ_0)-minimum-norm solution $(\kappa^\dagger, \mu^\dagger)$, i.e., a solution which is compatible with the data and has minimal distance to the a-priori guess (κ_0, μ_0). Under an additional assumption (cf. Theorem 4.7), this generalized solution can be shown to be locally unique [12].

The following results follow with minor modifications from standard regularization theory for nonlinear inverse problems, and we state them without proof. For details and proofs we refer to [13] or [12, Ch. 10]. Existence of minimizers, which is required for the well definedness of the regularization method, is a direct consequence of Theorem 3.5.

THEOREM 4.3 (existence of a minimizer). *For any $\alpha > 0$ the Tikhonov functional J_α has a minimizer in $\mathcal{D}(F)$.*

The next result states that the regularized solutions depend continuously on the data, as long as the regularization parameter is strictly positive.

THEOREM 4.4 (stability). *Let $\alpha > 0$, and let $\{y_n\}$ be a sequence of data with $y_n \to y$. Moreover, let (κ_n, μ_n) denote minimizers of* (12) *with y^δ replaced by y_n. Then $\{(\kappa_n, \mu_n)\}$ has a convergent subsequence, and the limit of every convergent subsequence is a minimizer of J_α in $\mathcal{D}(F)$.*

If the perturbations of the data go to zero and the regularization parameter is chosen appropriately, then the regularized solutions can be shown to converge.

THEOREM 4.5 (convergence). *Let $\{y_n\}$ denote a sequence of data with $\|y_n - y\| \leq \delta_n$. If $\delta_n \to 0$ and the regularization parameter is chosen such that $\alpha(\delta_n) \sim \delta_n$, then any sequence of minimizers $\{(\kappa_n, \mu_n)\}$ of the Tikhonov functional* (12) *with y^δ replaced by y_n contains a convergent subsequence, and the limit of every convergent subsequence is a (κ_0, μ_0)-minimum-norm solution of* (11).

In order to obtain quantitative convergence results, a source condition, i.e., some smoothness of the solution, is required. For stating such a condition, let us introduce the adjoint of the derivative operator $F'(\kappa, \mu)$; cf. Theorem 3.15. The following representation can be derived with standard arguments.

THEOREM 4.6 (adjoint problem). *Let $(\kappa, \mu) \in \mathcal{D}(F)$. Then the adjoint of the operator $F'(\kappa, \mu)$ defined in Theorem* 3.15 *is given by*

$$\begin{aligned} F'(\kappa, \mu)^*\colon L^2(\partial\Omega) &\to H^1(\Omega) \times L^2(\Omega), \\ r &\mapsto \big(d\kappa, d\mu\big), \end{aligned}$$

where $d\kappa \in H^1(\Omega)$ and $d\mu \in L^2(\Omega)$ are defined by $d\mu := -\overline{\Phi} R$ and

$$-\Delta d\kappa + d\kappa = -\nabla\overline{\Phi}\nabla R \quad \text{in } \Omega, \qquad \partial_n d\kappa = 0 \quad \text{on } \partial\Omega.$$

Here, Φ denotes the solution of the forward problem (1)–(2), *and R is the solution of the adjoint problem*

$$-\operatorname{div}(\kappa\nabla R) + (\mu - ik)R = 0 \qquad \text{in } \Omega, \tag{13}$$

$$\kappa\partial_n R + \rho R = \rho r \qquad \text{on } \partial\Omega. \tag{14}$$

For the following classical convergence rate result (cf. [13] or [12, Thm. 10.4]), it is usually assumed that F is Fréchet differentiable, with Lipschitz continuous Fréchet derivative. This condition can be replaced by the second order Taylor estimate stated in Theorem 3.16, and we obtain the following quantitative result.

THEOREM 4.7. *Let y^δ satisfy $\|y - y^\delta\| \leq \delta$, and let the assumptions of Theorem* 3.16 *hold. Assume that $(\kappa^\dagger, \mu^\dagger)$ is a (κ_0, μ_0)-minimum-norm solution and that the following conditions hold:*

1. *There exists an element $w \in L^2(\partial\Omega)$ such that*

$$(\kappa^\dagger, \mu^\dagger) - (\kappa_0, \mu_0) = Re\{F'(\kappa^\dagger, \mu^\dagger)^* w\}.$$

2. *There holds $C_L\|q\|_{2;\partial\Omega}\|w\| < 1$ with C_L from Theorem* 3.16.

Then for the parameter choice $\alpha = \delta$, we obtain the convergence rates

$$\|F(\kappa_\alpha^\delta, \mu_\alpha^\delta) - y^\delta\| = O(\delta) \quad \text{and} \quad \|(\kappa_\alpha^\delta, \mu_\alpha^\delta) - (\kappa^\dagger, \mu^\dagger)\| = O(\sqrt{\delta}).$$

Proof. Let us sketch the part of the proof, where the source condition comes into play: Let $x = (\kappa, \mu)$ abbreviate the pair of parameters and $(\cdot, \cdot)$, $\langle \cdot, \cdot \rangle$ denote the real, respectively, complex scalar products; i.e., $\langle a, b \rangle := (\overline{a}, b)$. Then we have

$$\begin{aligned}(x^\dagger - x_\alpha^\delta, x^\dagger - x_0) &= (x^\dagger - x_\alpha^\delta, \mathrm{Re}\{F'(x^\dagger)^* w\}) = \mathrm{Re}\langle x^\dagger - x_\alpha^\delta, F'(x^\dagger)^* w\rangle \\ &= \mathrm{Re}\langle F'(x^\dagger)(x^\dagger - x_\alpha^\delta), w\rangle.\end{aligned}$$

This term can then be further estimated by taking the absolute value and the Cauchy–Schwarz inequality. Apart from this slight modification, the proof is the same as the one of [12, Thm. 10.4]. ∎

Remark 4.8. For a numerical realization, the Tikhonov functional has to be minimized by some iterative algorithm. Such methods typically require the gradient of the Tikhonov functional, which in our case is given by [11]

$$\nabla J_\alpha(\kappa, \mu) = \mathrm{Re}\{F'(\kappa, \mu)^*[F'(\kappa, \mu) - y^\delta]\} + \alpha(\kappa - \kappa_0, \mu - \mu_0).$$

Note that one has to guarantee that the iterates stay in the convex set $\mathcal{D}(F)$, in order to ensure well definedness in the minimization process. Under the conditions of Theorem 4.7, one can show convergence of the projected iteratively regularized Gauß–Newton method; cf. [5, Thms. 4.1 and 4.2] or [25]. Further details on iterative methods for the problem under investigation, their discretization, and numerical results are presented in [11].

5. Summary. In this paper we established a rigorous analysis of the forward problem of diffuse optical tomography. In contrast to previous investigations of mapping properties of the forward operator in optical tomography, or, similarly, in electrical impedance tomography, we use Hilbert space topologies for the parameter space. This facilitates the numerical realization of the resulting regularization methods and allows the use of standard iterative algorithms for the solution of the corresponding nonlinear optimization problems. Besides showing the complete continuity of the forward operator, which implies the ill-posedness of the corresponding inverse problem, we also proved weak (sequential) closedness of the operator. This allows the stable solution by Tikhonov regularization (with Hilbert space penalty terms); i.p., the existence of minimizers for the Tikhonov functional is ensured. Moreover, convergence of minimizers towards a solution is guaranteed, if the noise level tends to zero and the regularization parameters are chosen appropriately. We also investigated differentiability of the forward operator and derived second order estimates for the remainder of the linear Taylor approximation, which allowed us to derive quantitative convergence rates estimates. Our results also allow us to apply iterative (regularization) methods for a numerical solution. For the analysis of the forward operator, we utilized $W^{1,p}$ regularity results for elliptic partial differential equations, which were derived in detail under minimal regularity assumptions on the parameters and mild smoothness requirements on the domain.

Appendix A. Let us start with a proof of Theorem 3.8 for the case $p_0 = 2$ and recall the definition of $\bar{p}$ and $\hat{p}$ given before the statement of Theorem 3.8.

THEOREM A1. *Let $\Omega \subset \mathbb{R}^d$, $d \geq 2$ be a Lipschitz domain, and let Assumption* 2.2 *hold. Then for every $f \in L^2(\Omega, \mathbb{R}^d)$, $g \in L^{\bar{2}}(\Omega)$, and $q \in L^{\hat{2}}(\partial\Omega)$, the problem* (8) *of Theorem* 3.8 *has a unique solution $u \in W^{1,2}(\Omega)$ that satisfies*

$$\|u\|_{1,2;\Omega} \leq C\big(\|f\|_{2;\Omega} + \|g\|_{\bar{2};\Omega} + \|q\|_{\hat{2};\partial\Omega}\big)$$

with a constant C depending only on the domain Ω and the bounds for the coefficients in Assumption 2.2.

Proof. By Hölder's inequality, we have

$$|(f,\nabla v)_\Omega + (g,v)_\Omega + (q,v)_{\partial\Omega}| \\ \leq \|f\|_{2;\Omega}\|v\|_{1,2;\Omega} + \|g\|_{(2^*)';\Omega}\|v\|_{2^*;\Omega} + \|q\|_{(2^\circ)';\partial\Omega}\|v\|_{2^\circ;\partial\Omega},$$

and application of embedding theorems (cf. Thm. 2.1), shows that the right-hand side of (8) defines a bounded linear functional on $H^1(\Omega)$. The result then follows from the complex version of the Lax–Milgram theorem [8, Ch. VII]. ∎

In order to generalize this theorem to the case $p_0 > 2$, we need the following basic results, which are a generalization of $W^{1,p}$ regularity results for Dirichlet problems [27, 35] to Neumann boundary conditions.

THEOREM A2. *Let $\Omega \subset \mathbb{R}^d$, $d \geq 2$ denote a domain with $\partial\Omega \in C^{1,1}$. Then for every $f \in L^p(\Omega,\mathbb{R}^d)$ and $g \in L^{\bar{p}}(\Omega)$, the problem*

$$(\nabla u, \nabla v)_\Omega + (u,v)_\Omega = (f,\nabla v)_\Omega + (g,v)_\Omega \qquad \textit{for all } v \in C^\infty(\overline{\Omega}) \tag{15}$$

has a unique solution $u \in W^{1,p}(\Omega)$ that satisfies

$$\|u\|_{1,p;\Omega} \leq C(\|f\|_{p;\Omega} + \|g\|_{\bar{p};\Omega}) \tag{16}$$

with a constant $C = C(p,\Omega)$ which is independent of the data f and g.

Proof. According to [33, Thm. 3.1], there exists a constant $C = C(p,\Omega)$ such that

$$\|u\|_{1,p;\Omega} \leq C(\|\Delta u\|'_{-1,p;\Omega} + \|u\|_{0,p;\Omega})$$

for all functions $u \in C^\infty(\overline{\Omega})$. Here $\|\cdot\|'_{-1,p;\Omega}$ denotes the norm of the dual space $\widetilde{W}^{-1,p}(\Omega) := \big(W^{1,p'}(\Omega)\big)'$. The result then follows by continuous embedding of Sobolev spaces; cf. Thm. 2.1. ∎

Remark A3. The previous result is based on $W^{2,p}$ regularity of solutions of the Neumann problem $-\Delta u + u = f$ (cf. [17, Prop. 2.5.2.3]), which requires a $C^{1,1}$ boundary. The estimate (16) can then be derived by interpolation arguments; cf. [33]. In view of the results of [35, Thm. 4.6], we conjecture that a C^1-regular boundary should be sufficient for the result to hold.

The following results are derived with the arguments of [19], where nonlinear mixed boundary value problems were considered. In order to keep track of the assumptions and constants, we carry out the derivations in detail for our linear problem.

Because of Theorem A2, the mapping $J{:}W^{1,p}(\Omega) \to \widetilde{W}^{-1,p}(\Omega)$ defined by $\langle Ju, v\rangle := \int_\Omega \nabla\overline{u}\nabla v + \overline{u}v\,dx$ for $v \in W^{1,p'}(\Omega)$ is an isomorphism, and the norm of its inverse is given by

$$M_p := \sup\{\|u\|_{1,p;\Omega} : u \in W^{1,p}(\Omega),\ \|Ju\|'_{-1,p} \leq 1\}.$$

Note that by the Riesz representation theorem $M_2 = 1$. The linear mapping L: $W^{1,p}(\Omega) \to Y_p := L^p(\Omega,\mathbb{R}^{d+1})$, $u \mapsto (u,\nabla u)$ is continuous. By identifying Y_p with its dual, the adjoint L^* maps Y_p continuously into $\widetilde{W}^{-1,p}(\Omega)$, and there holds $J = L^*L$. Let us define $A{:}W^{1,p}(\Omega) \to \widetilde{W}^{-1,p}(\Omega)$ by $\langle Au, v\rangle := \int_\Omega \kappa\nabla\overline{u}\nabla v + c\overline{u}v\,dx$ for $v \in W^{1,p'}(\Omega)$ with constant $c := \sqrt{\underline{\kappa}\overline{\kappa}}$.

THEOREM A4. *Let Ω be of class $C^{1,1}$. If $l := \frac{\overline{\kappa}-\underline{\kappa}}{\underline{\kappa}+\overline{\kappa}} < 1/M_p$, then A is an isomorphism between $W^{1,p}(\Omega)$ and $\widetilde{W}^{-1,p}(\Omega)$. In particular, for every $h \in \widetilde{W}^{-1,p}(\Omega)$, the variational problem*

$$\langle Au, v\rangle = \langle h, v\rangle \qquad \textit{for all } v \in W^{1,p'}(\Omega)$$

has a unique solution $u \in W^{1,p}(\Omega)$ *that satisfies* $\|u\|_{1,p;\Omega} \le C\|h\|'_{-1,p;\Omega}$ *with constant* C *depending only on* Ω, p, *and the bounds on the coefficients.*

Proof. Compare to the proof of [19, Thm. 1]. For $t = \frac{2}{\overline{\kappa}+\underline{\kappa}}$, the operator $T{:}Y_p \to Y_p$, $y = (y_0, y') \mapsto y - t(cy_0, \kappa y')$ is Lipschitz continuous with constant $l < 1/M_p$; moreover, there holds $L^*TL = J - tA$. The mapping $Q_h{:}W^{1,p}(\Omega) \to W^{1,p}(\Omega)$ defined by $Q_h u := J^{-1}(L^*TLu + th) = u - tJ^{-1}(Au - h)$ satisfies $\|Q_h u_1 - Q_h u_2\|_{1,p;\Omega} \le M_p l \|u_1 - u_2\|_{W^{1,p}(\Omega)}$; i.e., Q_h is Lipschitz continuous with Lipschitz constant $lM_p < 1$ (independent of h). The result then follows with Banach's fixed point theorem. ☐

Remark A5. Even for nonsmooth domains, the result holds at least for some $p > 2$; cf. [19]. Note that $l < 1$, and thus $lM_p < 1$ for p sufficiently close to 2 since $M_p \to 1$ as $p \to 2$.

Proof of Theorem 3.8. The problem of Theorem 3.8 can be written as

$$\begin{aligned}(\kappa\nabla u, \nabla v)_\Omega + c(u, v)_\Omega = ((c - \mu - ik)u, v)_\Omega - (\rho u, v)_{\partial\Omega}\\ + (f, \nabla v)_\Omega + (g, v)_\Omega + (\rho q, v)_{\partial\Omega} =: \langle h, v\rangle,\end{aligned}$$

where $c := \sqrt{\overline{\kappa}\underline{\kappa}}$ is defined as above. Let us consider the case $2 \le p \le 3$ first (which is the relevant case for the analysis of section 3), and assume that the conditions of Theorem A4 hold. It remains to show that h is a bounded linear functional on $W^{1,p'}(\Omega)$ that can be estimated appropriately. By Hölder's inequality and embedding theorems (cf. Thm. 2.1), we obtain

$$\begin{aligned}|\langle h, v\rangle| &\le C'(\|u\|_{6;\Omega} + \|u\|_{4;\partial\Omega} + \|f\|_{p;\Omega} + \|g\|_{\bar{p};\Omega} + \|q\|_{\hat{p};\partial\Omega})\|v\|_{1,p';\Omega}\\ &\le C(\|f\|_{p;\Omega} + \|g\|_{\bar{p};\Omega} + \|q\|_{\hat{p};\partial\Omega})\|v\|_{1,p';\Omega},\end{aligned}$$

where the last inequality follows from Theorem A1. The result then follows from Theorem A4. Having established this higher regularity of solutions u, the case $p > 3$ can be treated by a bootstrapping argument. The case $p \le 2$ follows with the standard duality arguments. Thus for smooth domains, and $\overline{\kappa}/\underline{\kappa}$ sufficiently close to 1, Theorem 3.8 holds for any $p_0 < \infty$. For nonsmooth domains, or $\overline{\kappa} \gg \underline{\kappa}$, the theorem follows from the results of [19] and Remark A5 at least for some $p_0 > 0$. ☐

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