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THE FORWARD AND INVERSE PROBLEM IN  
REFRACTIVE INDEX BASED OPTICAL TOMOGRAPHY**

By

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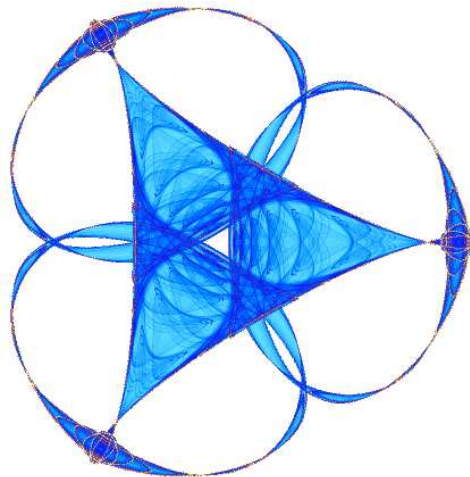
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# ON EXISTENCE AND UNIQUENESS OF THE FORWARD AND INVERSE PROBLEM IN REFRACTIVE INDEX BASED OPTICAL TOMOGRAPHY\*

TAUFIQUAR KHAN , ALAN THOMAS , AND JEONG-ROCK YOON

**Abstract.** In optical tomography, conventionally the diffusion approximation (DA) to the radiative transport equation (RTE) with a constant refractive index is used. The existence, uniqueness, and non-uniqueness of the forward and the inverse problem using conventional DA has been studied in the past. In this report, we investigate the existence, uniqueness, and non-uniqueness of optical tomography forward and the inverse problem based on the DA to the RTE for a highly scattering medium with a spatially varying refractive index. We establish criteria for existence and uniqueness of solutions. In particular, we derive a nonlinear partial differential equation for the parameter constraint whose unique solvability guarantees uniqueness of the inverse problem.

**Key words.** existence, uniqueness, elliptic pdes, inverse problems, optical tomography, refractive index, highly scattering media, turbid media, radiative transport, and biomedical imaging.

**1. INTRODUCTION.** Media with spatially varying refractive index are among us in the form of biological tissues and the atmosphere [13, 11]. Modelling photon transport in such media is potentially better done when these variations are taken into account. Additionally, spatially resolved estimations of refractive index may provide a means to distinguish between two types of such media, e.g. two kinds of human tissue. This potential has prompted recent interest in the radiative transport equation (RTE) for a medium with spatially varying refractive index [9, 10, 14, 8].

In optical tomography, conventionally the diffusion approximation DA to the RTE with a constant refractive index is used. The existence, uniqueness, and non-uniqueness of the forward and the inverse problem using the conventional DA has been studied extensively in the past [2, 3]. In this report, we investigate the existence, uniqueness, and non-uniqueness of the optical tomography forward and inverse problems based on the DA to the RTE for a highly scattering medium with a spatially varying refractive index. We establish criteria for existence and uniqueness of solutions.

Let  $\Omega \subset \mathbb{R}^d$  ( $d = 2$  or  $d = 3$ ) be simply connected, open, and bounded with boundary  $\partial\Omega$  which is  $C^2$ . Let  $\mu_a \in L^\infty(\Omega)$ ,  $\tilde{f} \in H^{-\frac{1}{2}}(\partial\Omega)$ , and  $n, D \in H^2(\Omega)$ . Then the diffusion approximation to the radiative transfer equation (RTE) with spatially varying refractive index is given by [9, 10]:

$$(1.1) \quad \left( \frac{n(x)}{c_0} \frac{\partial}{\partial t} + \mu_a(x) \right) v(x, t) - \nabla \cdot \left[ D(x) \left( \nabla - \frac{2}{n(x)} \nabla n(x) \right) v(x, t) \right] = 0 \quad \text{in } \Omega$$

with the Robin boundary condition

$$(1.2) \quad v + 2D \left( \frac{\partial}{\partial \nu} - \frac{2}{n} \frac{\partial n}{\partial \nu} \right) v = \tilde{f} \quad \text{on } \partial\Omega$$

and Neumann measurement

$$(1.3) \quad \tilde{g} = -2D \frac{\partial v}{\partial \nu} \quad \text{on } \partial\Omega$$

where  $\nu(x)$  denotes the outward unit normal to  $\partial\Omega$ ,  $n(x)$  is the spatially varying refractive index coefficient,  $c = c_0$  is the constant speed of light in vacuum,  $D(x)$  is the diffusion coefficient, and  $\mu_a(x)$  is the absorption coefficient. Here we assume that all of these parameters are time independent.

In optical tomography, there are three types of experiments [2]: (i) in the time domain, (ii) in the frequency domain, and (iii) the time independent or DC case. In time domain, typically delta type laser pulse  $\tilde{f}$  is used to generate the diffusion waves through the medium to be measured at the detectors and the full parabolic model (1.1) should be used. In the frequency domain, a frequency ( $\omega$ ) modulated laser pulse is used to probe the media and in the time independent case, only continuous waves are sent by laser. In our analysis, we will mainly consider frequency domain and DC optical tomography models. In fact, we will

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only consider frequency domain case and the DC case will automatically follow as  $\omega = 0$  case. Therefore, we take the time domain Fourier transform of equations (1.1)-(1.3) and we get the following:

$$(1.4) \quad -\nabla \cdot \left[ D \left( \nabla - \frac{2}{n} \nabla n \right) u \right] + \left( \mu_a + \frac{i\omega n}{c_0} \right) u = 0 \quad \text{in } \Omega$$

with the following boundary condition

$$(1.5) \quad u + 2D \left( \frac{\partial}{\partial \nu} - \frac{2}{n} \frac{\partial n}{\partial \nu} \right) u = \hat{f} \quad \text{on } \partial\Omega$$

and the following Neumann measurement

$$(1.6) \quad \hat{g} = -2D \frac{\partial u}{\partial \nu} \quad \text{on } \partial\Omega$$

where  $\partial/\partial t$  has been replaced by  $i\omega$  and  $u = u(x, \omega) = \mathcal{F}[v(x, t)]$  and  $\hat{f} = \hat{f}(x, \omega) = \mathcal{F}[\tilde{f}(x, t)]$ ,  $\hat{g} = \hat{g}(x, \omega) = \mathcal{F}[\tilde{g}(x, t)]$  are the corresponding Fourier transforms.

Now, we can define the forward problem as: given sources  $\hat{f}_j$  on  $\partial\Omega$  and a vector of model parameters  $q$  in  $Q$ , for example the coefficient of diffusion  $D$ , spatially varying refractive index  $n$ , and the coefficient of absorption  $\mu_a$  (i.e.  $q = (D, n, \mu_a)^T$ ) that belongs to a parameter set  $Q$ , find the data  $\hat{g}_j$  on  $\partial\Omega$ . The associated inverse problem is defined as: given sources  $\hat{f}_j$  and data  $\hat{g}_j$  on  $\partial\Omega$  find the  $q$  in  $Q$ , that yields this data. In the literature, typically there are two approaches for analysis of the inverse problem: (i) output least square formulation [4] and (ii) Dirichlet-to-Neumann (DtoN) formulation [12]. In this report, we will address both formulation, in section 3, we will investigate output least square formulation and in section 4, we will investigate the DtoN formulation. The outline of the report is as follows. In section 2, we will investigate the existence and uniqueness of the forward problem. In section 3, we will investigate the existence of the least square inverse problem. In section 4, we will investigate uniqueness and non-uniqueness of the inverse problem. In section 5, we discuss the future direction of our work.

**2. EXISTENCE AND UNIQUENESS OF THE FORWARD PROBLEM.** We shall now devote our attention to the weak formulation of the boundary value problem

$$(2.1) \quad \begin{aligned} -\nabla \cdot \left[ D \left( \nabla - \frac{2}{n} \nabla n \right) u \right] + \left( \mu_a + \frac{i\omega n}{c_0} \right) u &= 0 \quad \text{in } \Omega \\ u + 2D \left( \frac{\partial}{\partial \nu} - \frac{2}{n} \frac{\partial n}{\partial \nu} \right) u &= \hat{f} \quad \text{on } \partial\Omega. \end{aligned}$$

We work primarily in  $H^1(\Omega) = W^{1,2}(\Omega)$  the Sobolev space of degree 2 and order 1. Define the inner product  $\langle \cdot, \cdot \rangle_V$  by

$$(2.2) \quad \langle u, \phi \rangle_V := \langle \nabla u, \nabla \phi \rangle_{L^2(\Omega)} + \langle u, \phi \rangle_{L^2(\partial\Omega)}$$

It is well known that the induced norm  $\| \cdot \|_V$ , given by

$$(2.3) \quad \|u\|_V := \left( \|\nabla u\|_{L^2(\Omega)}^2 + \|u\|_{L^2(\partial\Omega)}^2 \right)^{\frac{1}{2}},$$

is an equivalent norm to  $\| \cdot \|_{H^1(\Omega)}$  [1, 5]. When using  $\| \cdot \|_V$ , we will denote  $H^1(\Omega)$  by  $V(\Omega)$ .

The weak form of (2.1) is obtained by multiplying both sides by a test function  $\phi(x)$  and integrating over the spatial domain  $\Omega$ :

$$\int_{\Omega} \left( \mu_a + \frac{i\omega n}{c_0} \right) u \phi dx - \int_{\Omega} \nabla \cdot \left[ D \left( \nabla - \frac{2}{n} \nabla n \right) u \right] \phi dx = 0.$$

Integrating by parts and applying the boundary condition yields

$$(2.4) \quad \int_{\Omega} D \left( \nabla - \frac{2}{n} \nabla n \right) u \cdot \nabla \phi dx + \int_{\Omega} \left( \mu_a + \frac{i\omega n}{c_0} \right) u \phi dx + \frac{1}{2} \int_{\partial\Omega} u \phi ds = \frac{1}{2} \int_{\partial\Omega} \hat{f} \phi ds.$$

Now define the bilinear form  $B[\cdot, \cdot]$  by

$$(2.5) \quad B[u, \phi] = \int_{\Omega} D \nabla u \cdot \overline{\nabla \phi} dx - \int_{\Omega} \left( D \frac{2}{n} \nabla n \right) u \cdot \overline{\nabla \phi} dx + \int_{\Omega} \left( \mu_a + \frac{i\omega n}{c_0} \right) u \overline{\phi} dx + \frac{1}{2} \int_{\partial\Omega} u \overline{\phi} ds.$$

Then we may express (2.4) as

$$(2.6) \quad B[u, \phi] = F(\phi) \quad \text{for all } \phi \in V(\Omega)$$

where

$$F(\phi) := \frac{1}{2} \int_{\partial\Omega} \hat{f} \overline{\phi} ds.$$

Note that  $F$  is a bounded linear functional on  $H^1(\Omega)$ , because  $\hat{f} \in H^{-\frac{1}{2}}(\partial\Omega)$  and  $\phi|_{\partial\Omega} \in H^{\frac{1}{2}}(\partial\Omega)$ . We will proceed to verify the continuity and coercivity conditions of the Lax-Milgram lemma (see [6]) for the form  $B[\cdot, \cdot]$ , thus showing that (2.4) has a unique solution  $u \in V$  for all  $\phi \in V$ .

Suppose that  $0 < b_1 \leq D \leq a_1$ ,  $0 < \mu_a$ ,  $\|\mu_a + \frac{i\omega n}{c_0}\|_{\infty} \leq a_2$ , and that  $\|\frac{2}{n} \nabla n\|_{\infty} \leq a_3$ . Also let  $a_4$  satisfy  $\|\phi\|_{L^2(\Omega)} \leq a_4 \|\phi\|_V$  for all  $\phi \in V$ . Further assume that  $\min\{b_1, 1/2\} > a_1 a_3 a_4$ .

### 2.1. Continuity.

$$|B[u, \phi]| \leq a_1 \int_{\Omega} |\nabla u \cdot \overline{\nabla \phi}| dx + a_1 a_3 \int_{\Omega} |u| \cdot |\overline{\nabla \phi}| dx + a_2 \int_{\Omega} |u \overline{\phi}| dx + \frac{1}{2} \int_{\partial\Omega} |u \overline{\phi}| ds.$$

Applying Hölder's inequality we get

$$\begin{aligned} |B[u, \phi]| &\leq a_1 \left( \int_{\Omega} |\nabla u|^2 dx \right)^{1/2} \left( \int_{\Omega} |\nabla \phi|^2 dx \right)^{1/2} + a_1 a_3 \left( \int_{\Omega} |u|^2 dx \right)^{1/2} \left( \int_{\Omega} |\nabla \phi|^2 dx \right)^{1/2} \\ &\quad + a_2 \left( \int_{\Omega} |u|^2 dx \right)^{1/2} \left( \int_{\Omega} |\phi|^2 dx \right)^{1/2} + \frac{1}{2} \left( \int_{\partial\Omega} |u|^2 ds \right)^{1/2} \left( \int_{\partial\Omega} |\phi|^2 ds \right)^{1/2} \\ &\leq a_1 \left( \|\nabla u\|_{L^2(\Omega)}^2 + \|u\|_{L^2(\partial\Omega)}^2 \right)^{1/2} \left( \|\nabla \phi\|_{L^2(\Omega)}^2 + \|\phi\|_{L^2(\partial\Omega)}^2 \right)^{1/2} \\ &\quad + a_1 a_3 \|u\|_{L^2(\Omega)} \left( \|\nabla \phi\|_{L^2(\Omega)}^2 + \|\phi\|_{L^2(\partial\Omega)}^2 \right)^{1/2} + a_2 \|u\|_{L^2(\Omega)} \|\phi\|_{L^2(\Omega)} \\ &\quad + \frac{1}{2} \left( \|\nabla u\|_{L^2(\Omega)}^2 + \|u\|_{L^2(\partial\Omega)}^2 \right)^{1/2} \left( \|\nabla \phi\|_{L^2(\Omega)}^2 + \|\phi\|_{L^2(\partial\Omega)}^2 \right)^{1/2} \\ &\leq \left( a_1 + a_1 a_3 a_4 + a_2 a_4^2 + \frac{1}{2} \right) \|u\|_V \|\phi\|_V. \end{aligned}$$

Letting  $\alpha = (a_1 + a_1 a_3 a_4 + a_2 a_4^2 + \frac{1}{2})$  we obtain  $|B[u, \phi]| \leq \alpha \|u\|_V \|\phi\|_V$  as desired.

### 2.2. Coercivity.

Now consider

$$\begin{aligned} \operatorname{Re}(B[u, u]) &= \int_{\Omega} D |\nabla u|^2 dx - \int_{\Omega} \left( D \frac{2}{n} \nabla n \right) u \cdot \nabla u dx + \int_{\Omega} \mu_a |u|^2 dx + \frac{1}{2} \int_{\partial\Omega} |u|^2 ds \\ &\geq \min \left\{ b_1, \frac{1}{2} \right\} \|u\|_V^2 - \int_{\Omega} \left( D \frac{2}{n} \nabla n \right) u \cdot \nabla u dx + \int_{\Omega} \mu_a |u|^2 dx. \end{aligned}$$

Taking note that  $\mu_a(x) \geq 0$  for all  $x \in \Omega$  we may neglect the last integral and write

$$\operatorname{Re}(B[u, u]) \geq \min \left\{ b_1, \frac{1}{2} \right\} \|u\|_V^2 - \int_{\Omega} D \frac{2}{n} \nabla n u \cdot \nabla u dx.$$

Using Hölder's inequality to estimate the second integral, we get:

$$\begin{aligned} \operatorname{Re}(B[u, u]) &\geq \min \left\{ b_1, \frac{1}{2} \right\} \|u\|_V^2 - a_1 a_3 \left( \int_{\Omega} |u|^2 dx \right)^{1/2} \left( \int_{\Omega} |\nabla u|^2 dx \right)^{1/2} \\ &\geq \min \left\{ b_1, \frac{1}{2} \right\} \|u\|_V^2 - a_1 a_3 a_4 \|u\|_V^2 \\ &\geq \left( \min \left\{ b_1, \frac{1}{2} \right\} - a_1 a_3 a_4 \right) \|u\|_V^2. \end{aligned}$$

Letting  $\beta = \min\{b_1, 1/2\} - a_1 a_3 a_4$ , we obtain

$$\beta \|u\|_V^2 \leq \operatorname{Re}(B[u, u]).$$

Having satisfied the continuity and coercivity conditions of the Lax-Milgram lemma, we conclude that the boundary value problem (2.1) has a unique solution  $u$  which satisfies the a priori estimate

$$(2.7) \quad \|u\|_{L^2(\Omega)}^2 + \|u\|_{L^2(\partial\Omega)}^2 \leq C \|\hat{f}\|_{L^2(\partial\Omega)}^2$$

for some constant  $C > 0$  which is dependent only on the parameters  $D, n$  and  $\mu_a$ . Otherwise stated, the solution is continuous with respect to data.

**3. OUTPUT LEAST SQUARE FORMULATION OF THE INVERSE PROBLEM.** In this section we shall concern ourselves with the existence of local solutions that minimize a particular cost functional, which is important to computational methods. In general, measurement of  $u(q)$  may not be possible, only some observable part  $\mathcal{C}u(q)$  of the actual state  $u(q)$  may be measured. In this abstract setting, the objective of the inverse or parameter estimation problem is to choose a parameter  $q^*$  in  $Q$ , that minimizes an error criterion or cost functional  $J(u(q), \mathcal{C}u(q), q)$  over all possible  $q$  in  $Q$  subject to  $u(q)$  satisfying the diffusion approximation. A typical observation operator is,

$$(3.1) \quad \mathcal{C}^f u(q) = \left\{ -D \frac{\partial u}{\partial \nu}(x_i; q, f) \right\}_{i=1}^m$$

where  $x_i$  is in  $\partial\Omega$ ,  $m$  is the number of measurements. A typical cost functional  $J_\lambda$  is given as,

$$(3.2) \quad J_\lambda(q) = \frac{1}{2} \sum_{j=1}^{m_s} \sum_{i=1}^m \left| \mathcal{C}_i^{f_j} u(q) - z_i^{f_j} \right|^2 + \lambda \|q - q_0\|^2$$

where  $z_i^{f_j}$  is the measured data at the boundary for a given source  $f_j$  and  $\lambda$  is the Tikhonov regularization parameter. Now composing  $u(q)$  and  $\mathcal{C}u(q)$  we obtain the parameter-to-output mapping:  $T[q] = \mathcal{C}u$ . This is the nonlinear mapping of refractive index based diffusion optical tomography in abstract setting.

In this section, we will define  $q$  as

$$q = (D, n, \mu_a)$$

Let  $Q = W^{1,p}(\Omega) \times W^{1,\infty}(\Omega) \times L^\infty(\Omega)$  where  $W^{k,p}$  is the standard Sobolev space with the norm  $\|\cdot\|_{W^{k,p}}$  and  $p > 1$ . Suppose  $Q_1$  is the subspace of  $Q$  such that

$$(3.3) \quad Q_1 = \{q \in Q : \|D\|_{W^{1,p}} \leq \alpha_1, \|n\|_{W^{1,\infty}} \leq \alpha_2, \|\mu_a\|_{L^\infty} \leq \alpha_3\}.$$

Now  $Q_1$  endowed with the topology

$$(3.4) \quad W_{weak}^{1,p} \times W_{weak}^{1,\infty} \times L_{weak^*}^\infty$$

is a metric space. This follows from the facts i)  $W_{weak}^{1,p}$  is metrizable because closed unit sphere of a reflexive Banach space is compact in weak topology and ii) the  $L_{weak^*}^\infty$  coordinates are metrizable because these coordinates can be shown to be compact using Alaoglu's theorem together with separability of  $L^1$ . If we further restrict our parameter set  $Q_1$  to the following

$$(3.5) \quad \tilde{Q} = \{q \in Q_1 : \|D\|_{W^{1,p}} \leq \alpha_1, \|n\|_{W^{1,\infty}} \leq \alpha_2, \bar{\mu} < \|\mu_a\|_{L^\infty} \leq \alpha_3\}.$$

It can be shown that  $\tilde{Q}$  is a compact subset of  $Q$ , we refer the reader to Lemma 1.3 p. 223 [4] for further details. It can also be shown that there exists unique weak solution  $u(q) \in H^1$  for all  $q \in \tilde{Q}$  and moreover there exists uniform continuity in  $H^1 \cap H^2$  with respect to data over  $\tilde{Q}$  mainly  $\|u(q)\|_{H^2} \leq K \|f\|_{L^2}$  where  $K$  is independent of  $q \in \tilde{Q}$ , see Corollary 1.1, p. 222 [4] and Lemma 1.4, p. 223 [4] for a proof.

**3.1. Continuity With Respect to Parameters.** Let  $\{q^k\}$  be a sequence in  $\tilde{Q}$  such that  $q^k \rightarrow q$ . We claim that  $q \in \tilde{Q}$  and  $u(q^k) \rightarrow u(q)$  weakly in  $H^2$ . The fact that  $q \in \tilde{Q}$  is obvious because we assume  $\tilde{Q}$  is compact and there is at least a subsequence  $q^{k_j}$  that converges to  $q$  in  $\tilde{Q}$ . Furthermore  $u(q)$  exists from the regularity of  $u(q)$  over  $\tilde{Q}$ . Now let  $u(q)$  satisfy the following weak formulation of the refractive index diffusion equation

$$(3.6) \quad \int_{\Omega} D \left( \nabla - 2 \frac{\nabla n}{n} \right) u(q) \cdot \nabla \phi dx + \int_{\Omega} \left( \mu_a + \frac{i\omega n}{c_0} \right) u(q) \phi dx + \frac{1}{2} \int_{\partial\Omega} u(q) \phi ds = \frac{1}{2} \int_{\partial\Omega} f \phi ds$$

and let  $u(q^k)$  satisfy the following weak formulation:

$$(3.7) \quad \int_{\Omega} D^k \left( \nabla - 2 \frac{\nabla n^k}{n} \right) u(q^k) \cdot \nabla \phi dx + \int_{\Omega} \left( \mu_a^k + \frac{i\omega n^k}{c_0} \right) u(q^k) \phi dx + \frac{1}{2} \int_{\partial\Omega} u(q^k) \phi ds = \frac{1}{2} \int_{\partial\Omega} f \phi ds.$$

Since we have uniform regularity of the solutions  $u(q^k)$  in  $\tilde{Q}$ , we have  $u(q^k)$  converges to some  $w \in H^1(\Omega)$  which satisfies equation (3.6). Furthermore because of our parameters in  $q^k$  are bounded both above and below by zero, we can approximate these functions by continuous functions and the fact that  $u_{x_i}(q^k)\phi$  is in  $L^1(\Omega)$ , we can take the limit in equation (3.7) and get (3.6). But the uniqueness of the solution to the refractive index diffusion approximation (see section 4), we deduce that  $u = w$  in  $H^1(\Omega)$ . Therefore we have shown that  $u(q^k) \rightarrow u(q)$ . This also guarantees that there exists a minimum of  $J(q)$  in equation (3.2) because the compactness of the parameter space  $\tilde{Q}$  combined with continuity of the solutions  $u(q)$  with respect to the parameters  $q \in \tilde{Q}$  as well as the fact that  $H^2(\Omega)$  is embedded in the space of continuous functions  $C(\Omega)$  and the fact that point evaluation of  $u(q)$  is a continuous operator.

**4. UNIQUENESS OF THE INVERSE PROBLEM USING DtN FORMULATION.** In this section, we will investigate the Dirichlet-to-Neumann formulation of the inverse problem. From (1.4)-(1.6), our frequency domain inverse problem is to determine  $(n, D, \mu_a) \in H^2(\Omega) \times H^2(\Omega) \times L^\infty(\Omega)$  from all possible Robin-to-Neumann pairs  $(\hat{f}, \hat{g}) \in H^{-1/2}(\partial\Omega) \times H^{-1/2}(\partial\Omega)$  which are related by the following boundary value problem, note that  $u \in H^1(\Omega)$ :

$$(4.1) \quad -\nabla \cdot (D\nabla u) + D\nabla \ln n^2 \cdot \nabla u + \left( \nabla \cdot (D\nabla \ln n^2) + \mu_a + \frac{i\omega n}{c_0} \right) u = 0 \quad \text{in } \Omega,$$

$$(4.2) \quad u + 2D \left( \frac{\partial}{\partial\nu} - \frac{2}{n} \frac{\partial n}{\partial\nu} \right) u = \hat{f} \quad \text{on } \partial\Omega,$$

$$(4.3) \quad \hat{g} = -2D \frac{\partial u}{\partial\nu} \quad \text{on } \partial\Omega.$$

Here we need an additional assumption that  $\frac{4D}{n} \frac{\partial n}{\partial\nu} \neq 1$  on  $\partial\Omega$ . Otherwise, the measurement information is nothing but the input information;  $\hat{g} = -\hat{f}$ .

Now, we will transform (4.1) to Schrödinger type equation and the Robin-to-Neumann boundary conditions (4.2)-(4.3) to Dirichlet-to-Neumann boundary conditions.

**4.1. Absorbing the first order term.** If we note that

$$\begin{aligned} n^2 \nabla \cdot \left( \frac{D}{n^2} \nabla u \right) &= n^2 \frac{1}{n^2} \nabla \cdot (D\nabla u) + n^2 D \nabla u \cdot \nabla \left( \frac{1}{n^2} \right) = \nabla \cdot (D\nabla u) - 2D \frac{\nabla n}{n} \cdot \nabla u \\ &= \nabla \cdot (D\nabla u) - D\nabla \ln n^2 \cdot \nabla u, \end{aligned}$$

then (4.1) becomes

$$(4.4) \quad -\nabla \cdot \left( \frac{D}{n^2} \nabla u \right) + \left( \frac{\nabla \cdot (D\nabla \ln n^2)}{n^2} + \frac{\mu_a}{n^2} + \frac{i\omega n}{c_0 n^2} \right) u = 0. \quad \text{in } \Omega.$$

**4.2. Converting to Schrödinger type equation.** If we further utilize the Liouville transformation  $w = \gamma u$  where  $\gamma := \frac{\sqrt{D}}{n}$ , then

$$\begin{aligned} \nabla \cdot \left( \frac{D}{n^2} \nabla u \right) &= \nabla \cdot \left( \frac{D}{n^2} \nabla \left( \frac{n}{\sqrt{D}} w \right) \right) \nabla \cdot \left( \gamma^2 \nabla \frac{w}{\gamma} \right) = \nabla \cdot [\gamma^2 \nabla (\gamma^{-1}) w + \gamma \nabla w] \\ &= \nabla \cdot (-w \nabla \gamma + \gamma \nabla w) = -w \Delta \gamma + \gamma \Delta w. \end{aligned}$$

Using this transformation (4.4) becomes

$$(4.5) \quad -\Delta w + \left( \frac{\Delta \gamma}{\gamma} + \frac{\nabla \cdot (D \nabla \ln n^2)}{D} + \frac{\mu_a}{D} + \frac{i\omega n}{c_0 D} \right) w = 0 \quad \text{in } \Omega$$

where we used the fact that  $n^2 \gamma^2 = D$ . On the other hand, we have

$$D \nabla \ln n^2 = n^2 \gamma^2 \nabla \ln n^2 = 2n \gamma^2 \nabla n = \gamma^2 \nabla n^2 = \gamma (\nabla (n^2 \gamma) - n^2 \nabla \gamma) = \gamma \nabla (n^2 \gamma) - (n^2 \gamma) \nabla \gamma.$$

From this we can simplify the sum of first two terms in the parenthesis of (4.5):

$$\frac{\Delta \gamma}{\gamma} + \frac{\nabla \cdot (D \nabla \ln n^2)}{D} \frac{\Delta \gamma}{\gamma} + \frac{\gamma \Delta (n^2 \gamma) - (n^2 \gamma) \Delta \gamma}{n^2 \gamma^2} = \frac{\Delta (n^2 \gamma)}{n^2 \gamma} = \frac{\Delta (n \sqrt{D})}{n \sqrt{D}}.$$

Hence (4.5) is now

$$(4.6) \quad -\Delta w + \left( \frac{\Delta (n \sqrt{D})}{n \sqrt{D}} + \frac{\mu_a}{D} + \frac{i\omega n}{c_0 D} \right) w = 0 \quad \text{in } \Omega.$$

**4.3. DtoN boundary condition.** We consider Dirichlet-to-Neumann boundary conditions for (4.6):

$$w = f, \quad \frac{\partial w}{\partial \nu} = g \quad \text{on } \partial \Omega.$$

We can find a linear relation between  $(\hat{f}, \hat{g})$  and  $(f, g)$  as follows: From (4.2) and (4.3), we have

$$(4.7) \quad \left( 1 - \frac{4D}{n} \frac{\partial n}{\partial \nu} \right) u + 2D \frac{\partial u}{\partial \nu} = \hat{f}, \quad -2D \frac{\partial u}{\partial \nu} = \hat{g} \quad \text{on } \partial \Omega.$$

Since  $w = \gamma u$ , we have

$$u = \frac{1}{\gamma} w = \frac{1}{\gamma} f, \quad \frac{\partial u}{\partial \nu} = \frac{\partial \gamma^{-1}}{\partial \nu} w + \frac{1}{\gamma} \frac{\partial w}{\partial \nu} = -\frac{1}{\gamma^2} \frac{\partial \gamma}{\partial \nu} f + \frac{1}{\gamma} g \quad \text{on } \partial \Omega.$$

Plugging the above into (4.7), we get the following linear relation;

$$\begin{pmatrix} \hat{f} \\ \hat{g} \end{pmatrix} = \begin{pmatrix} \frac{1}{\gamma} \left( 1 - \frac{4D}{n} \frac{\partial n}{\partial \nu} \right) - \frac{2D}{\gamma^2} \frac{\partial \gamma}{\partial \nu} & \frac{2D}{\gamma} \\ \frac{2D}{\gamma^2} \frac{\partial \gamma}{\partial \nu} & -\frac{2D}{\gamma} \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix}.$$

The determinant of the above matrix is  $-\frac{2D}{\gamma^2} \left( 1 - \frac{4D}{n} \frac{\partial n}{\partial \nu} \right) = -2n^2 \left( 1 - \frac{4D}{n} \frac{\partial n}{\partial \nu} \right) \neq 0$ , so the linear relation is also invertible, namely,

$$\begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} \gamma \left( 1 - \frac{4D}{n} \frac{\partial n}{\partial \nu} \right)^{-1} & \gamma \left( 1 - \frac{4D}{n} \frac{\partial n}{\partial \nu} \right)^{-1} \\ \frac{\partial \gamma}{\partial \nu} \left( 1 - \frac{4D}{n} \frac{\partial n}{\partial \nu} \right)^{-1} & \frac{\partial \gamma}{\partial \nu} \left( 1 - \frac{4D}{n} \frac{\partial n}{\partial \nu} \right)^{-1} - \frac{\gamma}{2D} \end{pmatrix} \begin{pmatrix} \hat{f} \\ \hat{g} \end{pmatrix}.$$

Therefore, knowing  $(\hat{f}, \hat{g})$  is equivalent to knowing  $(f, g)$  as long as  $n$  and  $D$  are known on  $\partial \Omega$ . Note  $f = w|_{\partial \Omega} \in H^{1/2}(\partial \Omega)$  although it is represented by a linear sum of  $\hat{f} \in H^{-1/2}(\partial \Omega)$  and  $\hat{g} \in H^{-1/2}(\partial \Omega)$ , since we already know  $w \in H^1(\Omega)$ . In summary, we have proved the following theorem.

**THEOREM 4.1.** *Assume  $n$  and  $D$  are known on  $\partial \Omega$  and satisfy  $\frac{4D}{n} \frac{\partial n}{\partial \nu} \neq 1$  on  $\partial \Omega$ . Then our frequency domain inverse problem is equivalent to determine  $(n, D, \mu_a) \in H^2(\Omega) \times H^2(\Omega) \times L^\infty(\Omega)$  from all possible*

Dirichlet-to-Neumann pairs  $(f, g) \in H^{1/2}(\partial\Omega) \times H^{-1/2}(\partial\Omega)$  which are related by the following Schrödinger type boundary value problem:

$$\begin{aligned} -\Delta w + \left( \frac{\Delta(n\sqrt{D})}{n\sqrt{D}} + \frac{\mu_a}{D} + \frac{i\omega n}{c_0 D} \right) w &= 0 \quad \text{in } \Omega, \\ w = f, \quad \frac{\partial w}{\partial \nu} &= g \quad \text{on } \partial\Omega. \end{aligned}$$

We will now deduce uniqueness conditions for the inverse problem which follow from the results of Sylvester and Uhlmann [12] and Grinberg [7] for the Schrödinger equation.

**THEOREM 4.2.** *Assume  $n$  and  $D$  are known on  $\partial\Omega$  and satisfy  $\frac{4D}{n} \frac{\partial n}{\partial \nu} \neq 1$  on  $\partial\Omega$ , and consider non-DC case ( $\omega \neq 0$ ). In 2D, we need an additional assumption that  $(n, D, \mu_a)$  are close to constants, while we do not need any extra assumptions in 3D. Then from the complete Dirichlet-to-Neumann data  $(f, g)$ , we can uniquely determine*

$$\frac{n}{D} =: \alpha \quad \text{and} \quad \frac{\mu_a}{D} + \frac{\Delta(n\sqrt{D})}{n\sqrt{D}} =: \beta \quad \text{in } \Omega.$$

Furthermore,  $\xi := n\sqrt{D}$  satisfies the following Dirichlet boundary value problem of nonlinear PDE;

$$(4.8) \quad \Delta \xi - \beta(x)\xi + \mu_a(x)[\alpha(x)]^{\frac{2}{3}}\xi^{\frac{1}{3}} = 0 \quad \text{in } \Omega, \quad \xi = n\sqrt{D} \quad \text{on } \partial\Omega.$$

*Proof.* From [12, 2] and [7], we know that the potential of Schrödinger equation is uniquely determined by the complete Dirichlet-to-Neumann map. So the real part,  $\beta$ , and the imaginary part,  $\omega\alpha/c_0$ , of the potential are individually determined.

Since  $\xi = n\sqrt{D}$  and  $\alpha = n/D$ , we have  $D = (\xi/\alpha)^{2/3}$ . Substituting it into the second equation, we get

$$0 = \Delta \xi - \beta \xi + \mu_a (\xi/\alpha)^{-2/3} \xi = \Delta \xi - \beta \xi + \alpha^{2/3} \mu_a \xi^{1/3}.$$

□

From the above theorem, we can readily deduce the following corollary for uniqueness in refractive index based optical tomography.

**COROLLARY 4.1.** *Under the same assumptions as in Theorem 4.2, we have the followings cases.*

(a) *If  $n$  is known, then  $D$  and  $\mu_a$  are uniquely determined as follows:*

$$D = \frac{n}{\alpha}, \quad \mu_a = \frac{\beta n}{\alpha} - \frac{\Delta(n^{3/2}/\sqrt{\alpha})}{\sqrt{\alpha n}}.$$

(b) *If  $D$  is known, then  $n$  and  $\mu_a$  are uniquely determined as follows:*

$$n = \alpha D, \quad \mu_a = \beta D - \frac{\Delta(\alpha D^{3/2})}{\alpha \sqrt{D}}.$$

(c) *If  $\mu_a$  is known then  $D$  and  $n$  are uniquely determined subject to the unique solvability of the nonlinear equations (4.8). Note also, when  $\mu_a = 0$  (non-absorbing medium), (4.8) is linear.*

*Proof.* (a) and (b) are obvious. For (c), once we have  $\xi = n\sqrt{D}$  and  $\alpha = n/D$ , we can uniquely determine  $n = (\alpha\xi^2)^{1/3}$  and  $D = (\xi/\alpha)^{2/3}$ . Note that when  $n(\mathbf{x}) \equiv 1$ , this result coincides with that of Arridge [2]. □

In our future works, to study the uniqueness of the inverse problem when  $\mu_a$  is known, we will investigate when (4.8) possess a unique solution.

**5. CONCLUSIONS AND DISCUSSIONS.** In summary, we derived a refractive index based optical tomography model, the inverse problem of which is to determine  $(n, D, \mu_a)$ . Through Dirichlet-to-Neumann formulation, we established two quantities that could be uniquely determined. In particular,  $(n, D, \mu_a)$  can be uniquely determined if either  $n$  or  $D$  is assumed to be known. When  $\mu_a$  is known, the unique identifiability is dependent on the unique solvability of the Dirichlet boundary value problem of a semilinear elliptic PDE. We are currently investigating this unique solvability condition and how we can take advantage of this condition as well as the nonlinear equation for the reconstruction of parameters.



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## REFERENCES

- [1] R. A. Adams and J.J.F. Fournier. *Sobolev Spaces*. Academic Press, Oxford, 2003.
- [2] S.R. Arridge. Optical tomography in medical imaging: Topical review. *Inverse Problems*, 15:R41–R93, 1999.
- [3] S.R. Arridge and W.R.B. Lionheart. Non-uniqueness in optical tomography. *Optics Lett.*, 23:882–884, 1998.
- [4] H.T. Banks and K. Kunisch. *Estimation Techniques for Distributed Parameter Systems*. Birkhauser, 2001.
- [5] D. Daners. Robin boundary value problems on arbitrary domains. *Transactions of the American Mathematical Society*, 352(9):4207–4236, 2000.
- [6] G. B. Folland. *Introduction to Partial Differential Equations 2nd edition*. Princeton University Press, Princeton, NJ, 1995.
- [7] N. I. Grinberg. Inverse boundary problem for the diffusion equation with the constant background: Investigation of uniqueness. *Fachbereich Mathematik und Informatik, Universität Münster, Münster, Germany*, 1998.
- [8] T. Khan and H. Jiang. A new diffusion approximation to the radiative transfer equation for scattering media with spatially varying refractive indices. *J. Opt. A: Pure Appl. Opt.*, 5:137–141, 2003.
- [9] T. Khan and A. Thomas. Comparison of  $p_n$  or spherical harmonics approximation for scattering media with spatially varying and spatially constant refractive indices. *Optics Communications*, 255:130–166, 2005.
- [10] T. Khan and A. Thomas. On derivation of the radiative transfer equation and its spherical harmonics approximation for scattering media with spatially varying refractive indices. *Clemson University Mathematical Sciences Technical Report*, TR2004-12-KT:1–49, December 2004.
- [11] MC Roggermann, BM Welsh, PJ Gardner, RL Johnson, and BL Pedersen. Sensing three-dimensional index-of-refraction variations by means of optical wavefront sensor measurements and tomographic reconstruction. *Optical Engineering*, 34(5):1374–1384, 1995.
- [12] J. Sylvester and G. Uhlmann. A global uniqueness theorem for an inverse boundary value problem. *Ann. Math.*, 125:153–169.
- [13] GJ Tearney, ME Brezinski, JF Southern, BE Bouma, MR Hee, and JG Fujimoto. Determination of the refractive index of highly scattering human tissue by optical coherence tomography. *Optics Letters*, 20(21):2258–2260, 1995.
- [14] J. Tualle and E. Tenet. Derivation of the radiative transfer equation for scattering media with spatially varying refractive index. *Optics Communications*, 228:33–38, 2003.