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Born expansion and Fréchet derivatives in nonlinear Diffuse Optical Tomography

Kiwoon Kwon [a,*], Birsen Yazıcı [b]

[a] Department of Mathematics, Dongguk University-Seoul, Seoul 100715, South Korea

[b] Electrical, Computer, and Systems Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180, USA

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ABSTRACT

The nonlinear Diffuse Optical Tomography (DOT) problem involves the inversion of the associated coefficient-to-measurement operator, which maps the spatially varying optical coefficients of turbid medium to the boundary measurements. The inversion of the coefficient-to-measurement operator is approximated by using the Fréchet derivative of the operator. In this work, we first analyze the Born expansion, show the conditions which ensure the existence and convergence of the Born expansion, and compute the error in the mth order Born approximation. Then, we derive the mth order Fréchet derivatives of the coefficient-to-measurement operator using the relationship between the Fréchet derivatives and the Born expansion.

1. Introduction

Diffuse Optical Tomography (DOT) in near infrared light is to determine the spatially resolved optical properties of a turbid medium from boundary measurements. The propagation of light is modeled by the photon diffusion equation in the frequency domain as follows [1]:

$$-\nabla \cdot (\kappa \nabla \Phi) + \left(\mu_a + \frac{\mathrm{i}\omega}{c}\right)\Phi = q \quad \text{in } \Omega, \tag{1.1a}$$

$$\Phi + 2a\nu \cdot (\kappa \nabla \Phi) = 0 \quad \text{on } \partial\Omega, \tag{1.1b}$$

where Ω is a Lipschitz domain in $\mathbb{R}^n$, $n = 2, \ldots$, $\partial\Omega$ is its boundary, c is the speed of light, q is the source term, ω is the angular frequency of the source q, ν is the unit outward normal vector on the boundary, Φ is the photon density function, and μ_a, μ_s', and $\kappa = \frac{1}{3(\mu_a+\mu_s')}$ are the absorption, reduced scattering, and diffusion coefficients, respectively. The constant a accounts for the refraction index mismatch at the boundary and we assume that a is a constant and κ, μ_a, and μ_s' are scalar functions satisfying

$$0 < L \le \kappa, \qquad \mu_a, \quad a \le U, \tag{1.2}$$

for some positive constants L and U.

Note that there are various definitions of the diffusion coefficient κ [2,3]. In this paper, we have followed the definition in [1].

* Corresponding author.
E-mail address: kwkwon@dongguk.edu (K. Kwon).

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For notational convenience, let

$$\mu = (\kappa, \mu_a). \tag{1.3}$$

Let us define coefficient-to-solution operator as

$$\Psi(\mu) = \Phi. \tag{1.4}$$

The inverse DOT problem is formulated as the inversion of the associated coefficient-to-measurement operator Γ, which maps the coefficients of the diffusion equation μ to the boundary measurements $\Gamma(\mu) = \Delta(\Phi) = \Delta(\Psi(\mu))$, where $\Delta(\Phi)$ can be either $\Phi|_{\partial\Omega}$(Born type) or $\log(\Phi|_{\partial\Omega})$(Rytov type) [1]. Thus, for the given boundary measurement Υ, the inverse DOT problem is to solve

$$\Gamma(\mu) = \Upsilon(\Phi), \tag{1.5}$$

or equivalently to solve the following minimization problem

$$\min_{\mu\in\mathcal{A}} \|\Gamma(\mu) - \Upsilon\|_{\mathcal{B}}, \tag{1.6}$$

for appropriate normed spaces $\mathcal{A}$ and $\mathcal{B}$. For the study of the unique determination of μ, see [4–6].

Let μ^0 be an initial guess for μ, then (1.5) is formally changed into

$$\Upsilon - \Gamma(\mu^0) = \Gamma'(\mu^0)(\delta\mu) + \frac{1}{2!}\Gamma''(\mu^0)(\delta\mu)^2 + \cdots, \tag{1.7}$$

where $\delta\mu = \mu^0 - \mu$ and $\Gamma', \Gamma'', \ldots$ are called the Fréchet derivatives of Γ.

Therefore, the inverse DOT problem is to find $\delta\mu$ by solving the nonlinear problem (1.7). Whereas, since (1.7) is represented by $\Upsilon - \Gamma(\mu^0) = \Gamma'(\mu^0)(\delta\mu) + O(\|\delta\mu\|^2_{\mathcal{B}})$, by neglecting higher order terms, we have a linearized inverse DOT problem to find a linear approximation $\delta\mu^L$ of $\delta\mu$ such that

$$\Upsilon - \Gamma(\mu^0) = \Gamma'(\mu^0)(\delta\mu^L). \tag{1.8}$$

Therefore, computing the Fréchet derivatives of the coefficient-to-measurement operator is an integral part for linearized and nonlinear DOT imaging. And, by definition, the Fréchet derivative of the coefficient-to-measurement operator Γ are closely related with the Fréchet derivative of the coefficient-to-solution operator Ψ, which will be addressed in detail in Section 4.2. The first order Fréchet derivative is used in (1.8), and to solve the nonlinear problem (1.7), the analysis for the higher order Fréchet derivatives are needed [7].

The following questions have to be addressed for the Eq. (1.7) to be meaningful:

- Do the Fréchet derivatives $\Gamma', \Gamma'', \Gamma''', \ldots$ (or $\Psi', \Psi'', \Psi''', \ldots$) exist? And what is appropriate normed spaces for the domain and codomain of Γ(or Ψ) for the Fréchet derivatives of Γ(or Ψ) exist?
- What are the conditions on $\delta\mu$ for the series expansion in the right hand side of (1.7) to converge to the left hand side of (1.7)?
- What is the approximation error between the finite series approximation of the right hand side of (1.7) and the left hand side of (1.7)?

We address the above questions by showing that the mth order Fréchet derivative of Ψ is the same as $m!$ times the mth order term in the Born expansion. Note that the Born expansion is the representation of the perturbed photon density by the unperturbed photon density and the perturbation in the optical coefficients.

To explain the Born expansion in detail, assume that μ is perturbed into $\widetilde{\mu}$ with $\widetilde{\mu} = \mu + \delta\mu$, and $\delta\kappa = 0$ in some neighborhood of $\partial\Omega$. Let the solution of (1.1) for the optical coefficients $\widetilde{\mu}$ be $\widetilde{\Phi}$. Then, we get the following equations:

$$-\nabla\cdot(\kappa\nabla\widetilde{\Phi}) + \left(\mu_a + \frac{\mathrm{i}\omega}{c}\right)\widetilde{\Phi} = q + \nabla\cdot(\delta\kappa\nabla\widetilde{\Phi}) - \delta\mu_a\widetilde{\Phi} \quad \text{in } \Omega, \tag{1.9a}$$

$$\widetilde{\Phi} + 2a\kappa\frac{\partial\widetilde{\Phi}}{\partial\nu} = 0 \quad \text{on } \partial\Omega. \tag{1.9b}$$

The solution of (1.1), Φ, is represented by the following integral equation:

$$\Phi(r) = \int_\Omega R(r, r')q(r')\mathrm{d}r', \tag{1.10}$$

where R is the Robin function. The detailed definition of the Robin function will be treated in Section 2. Likewise, the solution of (1.1), $\widetilde{\Phi}$, is represented by the following equation:

$$\widetilde{\Phi}(r) = \int_\Omega R(r, r')[q(r') + \nabla\cdot(\delta\kappa(r')\nabla\widetilde{\Phi}(r')) - \delta\mu_a(r')\widetilde{\Phi}(r')]\mathrm{d}r'. \tag{1.11}$$

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Using (1.10), (1.11), and by integration by parts, we obtain

$$\widetilde{\Phi}(\mathrm{r}) - \Phi(\mathrm{r}) = (\mathcal{R}\widetilde{\Phi})(\mathrm{r}), \tag{1.12}$$

where

$$\begin{aligned}
(\mathcal{R}\Psi)(\mathrm{r}) &= \mathcal{R}(\delta\mu)\Psi(\mathrm{r}) = (\mathcal{R}_1\Psi)(\mathrm{r}) + (\mathcal{R}_2\Psi)(\mathrm{r}),\\
(\mathcal{R}_1\Psi)(\mathrm{r}) &= \mathcal{R}_1(\delta\mu_a)\Psi(\mathrm{r}) = -\int_\Omega \delta\mu_a(\mathrm{r}')R(\mathrm{r},\mathrm{r}')\Psi(\mathrm{r}')\mathrm{dr}',\\
(\mathcal{R}_2\Psi)(\mathrm{r}) &= \mathcal{R}_2(\delta\kappa)\Psi(\mathrm{r}) = -\int_\Omega \delta\kappa(\mathrm{r}')\nabla R(\mathrm{r},\mathrm{r}')\nabla\Psi(\mathrm{r}')\mathrm{dr}'.
\end{aligned}$$

Using (1.12) recursively, we obtain the formal Born expansion:

$$\begin{aligned}
\widetilde{\Phi} &= \Phi + \mathcal{R}\widetilde{\Phi}\\
&= \Phi + \mathcal{R}\Phi + \mathcal{R}^2\widetilde{\Phi}\\
&= \cdots\\
&= \Phi + \mathcal{R}\Phi + \mathcal{R}^2\Phi + \cdots + \mathcal{R}^m\Phi + \mathcal{R}^{m+1}\widetilde{\Phi}\\
&= \Phi + \mathcal{R}\Phi + \mathcal{R}^2\Phi + \cdots.
\end{aligned} \tag{1.13}$$

The following questions have to be addressed for the Born expansion to be meaningful:

- What is the precise definition of the Robin function, and how singular is the Robin function around the source point?
- What are the conditions on the input function q for the Eq. (1.10) to be valid?
- For a given Ψ, is $\mathcal{R}^m$ defined for each m? What is the domain and codomain normed spaces (possibly Banach spaces) of the operator $\mathcal{R}^m\Psi$?
- What are the conditions on $\delta\mu$ for the infinite order Born expansion (the last expansion in (1.13) to converge)?
- How large is the error between $\widetilde{\Phi}$ and the mth order Born approximation? How does that error depend on Φ, μ and $\delta\mu$?

These questions will be addressed in Sections 2 and 3 and will be used to solve the questions for the Fréchet derivatives. It is evident that the formal Taylor expansion in (1.7) and the Born expansion have the same structures, and the mth order Fréchet derivatives of Γ and the mth order terms in the Born expansion have the same order of magnitude $O(\|\delta\mu\|_{\mathcal{B}}^m)$. In this paper, we solved the questions regarding the Fréchet derivatives by analyzing the corresponding questions in the Born expansion stated above and then showing that the mth order Fréchet derivatives of Ψ are the same as $m!$ times the mth order terms in the Born expansion, as in the following main theorem of this paper:

Theorem 1.1. *Let us define the coefficient-to-solution operator $\Psi : G \to B$ where normed space G and B are defined as follows:*

$$G = L^\infty(\Omega) \times L^\infty(\Omega), \qquad B = W^{1,p}(\Omega), \tag{1.14a}$$

$$G = L^\infty(\Omega), \qquad B = W^{1,p}(\Omega), \quad \textit{when } \delta\mu_a = 0, \tag{1.14b}$$

$$G = L^\infty(\Omega), \qquad B = L^p(\Omega), L^\infty(\Omega), W^{0,\infty}_{r,2}(\Omega), \quad \textit{or }, W^{0,\infty}_{r,\log}(\Omega), \quad \textit{when } \delta\kappa = 0, \tag{1.14c}$$

where the definition of the normed spaces will be given in Section 2. Then, the mth order Fréchet derivatives of Ψ is contained in $BL(G^m, B)$, or the space of the bounded linear operators from G^m to B, and are given by

$$\frac{\partial^m\Psi}{\partial\mu^m} = m!\mathcal{R}^m\Phi, \tag{1.15a}$$

$$\frac{\partial^m\Psi}{\partial\mu_a^k\partial\kappa^{m-k}} = m!\mathcal{R}_1^k\mathcal{R}_2^{m-k}\Phi. \tag{1.15b}$$

Even though the first order approximation of the Born expansion is widely used in the heuristic derivation of the first order Fréchet derivative (which was mentioned in [8]) in DOT, there are no studies regarding the derivation of Fréchet derivative as bounded linear operator between appropriate normed spaces in DOT [8,9], as far as we know. Thus, the present paper is the first paper deriving the mth order Fréchet derivative using the systematic study about the relationship between the Fréchet derivatives and the Born expansion.

A number of studies on the derivation of the Fréchet derivatives have been reported in inverse acoustic scattering problem [10–13] and in electrical impedance tomography [14,15]. In these studies, Fréchet derivatives are either given by the solution of partial differential equations using weak formulation [10,11,14,12] or by the solution of integral equation systems [15,13]. Although these studies, for example [10], are potentially applicable to DOT, most researchers in DOT use the perturbation method and the first order Born approximation to approximate the first order Fréchet derivative [1]. The heuristic derivation of the first order Fréchet derivative is straightforward; however, the higher order terms in the Born

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expansion are usually discarded regardless of the relative magnitude of the higher order terms with respect to the first order terms. Ye et al. [9] derived the Fréchet derivative of the coefficient-to-measurement operator using the perturbation method without using the first order Born approximation. However, in that work, the Robin function is assumed to be H^1 bounded, which is not valid. In contrast, in our work, we showed and used the argument that the convolution of the Robin function and any H^1 function is H^1 bounded [16,17]. Dierkes et al. [8] derived the first order Fréchet derivative for DOT, where a Dirichlet boundary problem with zero source is considered for the derivation, which is different from the model used in this paper.

The approach in this paper used in the derivation of the Fréchet derivatives differs from the approaches mentioned above [1,10,8,11,14,15,12,13,9]. We showed that the mth order Fréchet derivative is equal to the mth order term in the Born expansion up to constant multiples, whereas other approaches [10,8,11,14,15,12,13] do not provide any higher order derivatives. The approach using Born expansion for the derivation of the Fréchet derivative has several advantages over the previous approaches. First, the computation of the mth order Fréchet derivative is easier than the previous approaches, since we showed that the derivative is equal to $m!$ times the mth term in the Born expansion (1.15). Although Born expansion is well known in quantum and acoustic scattering and DOT [10,18–21,7,22–24], to the best of our knowledge, there has not been a study to relate the higher order Fréchet derivatives to the terms in Born expansion. Second, the recursive structure of the Born expansion makes it possible to bound the mth order Fréchet derivative in a variety of normed spaces by the mth multiple of the upper bound of the first order Fréchet derivative. Third, by using the relation between Fréchet derivatives and Born expansion, we can show that the inclusion of the higher order Fréchet derivatives improves the resolution of the reconstructed optical coefficients of DOT [7] and the upper bounds of the higher order Fréchet derivatives can be utilized in the convergence of the numerical DOT reconstruction algorithms [25] (See Section 4.3).

Studies on Born expansion were developed in the area of quantum scattering [26–31]. The analysis, in this paper, for the validity of the Born expansion and the error in the Born expansion differs from the analysis in quantum and acoustic scattering [10,26,18–22,29–31,23,24] in the following aspects. First, in these studies, the scattered wave is considered to be in an unbounded domain with spatially constant background properties of interest. Thus, the associated Green's function is explicitly known. However, we consider the Robin boundary condition for arbitrarily bounded domains and spatially varying background optical coefficients. Therefore, the existence, singularities, and other properties of the Robin function are not known a priori. Although the Green's function of the diffusion equation in specific geometries with specific optical coefficients is known analytically [32,7,33,34], to the best of our knowledge, studies on the existence and singularities of the Robin function for arbitrary geometries in which the Robin function is not known analytically have not been reported. Thus, we studied the properties about singularity of the Robin function using [16,17], based on the definition of the Robin function given in [35]. Second, in quantum and acoustic scattering theory, only the perturbation in the refractive index, which corresponds to the absorption coefficient in DOT, has been considered. In this work, we consider the perturbation with respect to both the absorption and reduced scattering coefficients. We note that the analysis of the Born expansion for the reduced scattering coefficient requires more sophisticated mathematical machinery as compared to the analysis of the Born expansion for the absorption coefficient. This complication results from the presence of the gradients of the Robin function and the unperturbed photon density in the Born expansion for the reduced scattering coefficient. Third, we establish a relationship between the Born expansion and the Fréchet derivatives of the coefficient-to-solution operator.

The rest of our paper is organized as follows: In Section 2, we provide a mathematical formulation of DOT. The definition, existence, and singular properties of the Robin function are given in Section 3. The validity of the Born expansion and the error analysis due to the mth order Born approximation is given in Section 4. In Section 5, we show that the Fréchet derivatives of the coefficient-to-solution operator are given by the terms in the Born expansion. Section 6 summarizes our results to make a conclusion. The paper concludes with two appendices providing proofs for Lemmas 2.2 and 3.6.

2. The Robin function

To explain the definition of the Robin function, we will introduce Sobolev spaces and weighted Sobolev spaces. To simplify our notation, for the rest of this paper, we will drop Ω from the definition of the function spaces. For example, we will use L^1 instead of $L^1(\Omega)$ for integrable functions on Ω. Let us define multi-index $\beta = (\beta_1, \beta_2, \dots, \beta_n)$, $|\beta| = \beta_1 + \beta_2 + \cdots + \beta_n$, and $D^\beta \phi = \frac{\partial^{|\beta|}}{\partial^{\beta_1} r_1 \, \partial^{\beta_2} r_2 \cdots \partial^{\beta_n} r_n}$ for nonnegative integers β_i, $i = 1, \dots, n$.

The Sobolev spaces and associated norms is as follows [36]:

$$L^p = \left\{ \phi \in L^1 \,|\, \|\phi\|_{L^p} := \left(\int_\Omega |\phi|^p \right)^{1/p} \leq \infty \right\},$$

$$W^{k,p} = \left\{ \phi \in L^p \,|\, \|\phi\|_{W^{k,p}} := \left(\sum_{l=0}^{k} \sum_{|\beta|=l} \left\| D^\beta \phi \right\|_{L^p}^p \right)^{1/p} \leq \infty \right\},$$

where $k = 1, 2, \dots, p \geq 1$ and

$$L^\infty = \{ \phi \in L^1 \,|\, \|\phi\|_{L^\infty} = \sup |\phi| \leq \infty \},$$

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$$W^{k,\infty} = \{\phi \in L^\infty | \, \|\phi\|_{W^{k,\infty}} = \max_{l=0,\dots,k} \max_{|\beta|=l} \left\| D^\beta \phi \right\|_{L^\infty} \le \infty\}.$$

It is well known that $W^{k,p}$ and $W^{k,\infty}$ are Banach spaces and $W^{k,\infty} \subset W^{k,p} \subset W^{k,q} \subset W^{k,1}$ for $p \ge q \ge 1$, since Ω is bounded. $W^{0,p} := L^p$ is called the Lebesgue space. In particular, $W^{k,2}$ is a Hilbert space and denoted by $W^{k,2} = H^k$. H^k is defined for noninteger and nonpositive values, such as $H^{-1}(\Omega)$ or $H^{1/2}(\partial\Omega)$. For the precise definition, see [36].

The weighted Sobolev spaces $W^{k,\infty}_{r_0,\alpha}$ and $W^{k,\infty}_{r_0,\log}$, for $r_0 \in \Omega$, a real number α, and the associated norms are given by:

$$W^{k,\infty}_{r_0,\alpha} = \{\phi | \, \|\phi\|_{W^{k,\infty}_{r_0,\alpha}} := \max_{l=0,\dots,k} \max_{|\beta|=l} \left\| |r - r_0|^{n-\alpha+l} D^\beta \phi \right\|_{L^\infty} < \infty\}, \tag{2.16a}$$

$$y_{r_0,\log} = \left\{ \phi | \, \|\phi\|_{W^{k,\infty}_{r_0,\log}} := \max \left(\max_{i=1,\dots,n} \left\| \frac{\partial \phi}{\partial r_i} \right\|_{W^{k-1,\infty}_{r_0,n}}, \left\| \frac{\phi(\cdot)}{\log(2d/|\cdot - r_0|)} \right\|_{L^\infty} \right) < \infty \right\}, \tag{2.16b}$$

where d is the maximum distance between two points contained in Ω. $W^{k,\infty}_{r_0,\alpha}$ and $W^{k,\infty}_{r_0,log}$ are also Banach spaces. For details about the weighted Sobolev spaces, see [37].

The followings hold for the Sobolev and weighted Sobolev spaces defined above:

$$\begin{aligned} &W^{k,\infty} \subset W^{k,\infty}_{r_0,\log}, \\ &W^{k,\infty}_{r_0,\alpha} \not\subseteq W^{k,1}, \quad \text{if } \alpha - k \le 0, \\ &W^{k,\infty} \subset W^{k,\infty}_{r_0,\alpha} \subset W^{k,1}, \ \text{if } \alpha - k > 0, \\ &W^{k,\infty} = W^{k,\infty}_{r_0,\alpha}, \quad \text{if } \alpha - k \ge n \end{aligned}$$

for $k = 0, 1, 2, \dots$.

Let us define the partial differential operators $\mathcal{M}$ and $\mathcal{N}$ on $H^1(\Omega)$ and $H^{1/2}(\partial\Omega)$, respectively, as follows:

$$\mathcal{M}\Psi = -\nabla \cdot (\kappa \nabla \Psi) + \left(\mu_a + \frac{\mathrm{i}\omega}{c} \right) \Psi \quad \text{for } \Psi \in H^1(\Omega), \tag{2.17a}$$

$$\mathcal{N}\psi = \psi + 2a\nu \cdot (\kappa \nabla \psi) \quad \text{for } \psi \in H^{1/2}(\partial\Omega). \tag{2.17b}$$

Then, (1.1) is represented by

$$\mathcal{M}\Phi = q \quad \text{in } \Omega, \tag{2.18a}$$

$$\mathcal{N}\Phi = 0 \quad \text{in } \partial\Omega. \tag{2.18b}$$

If there is a need to stress the operators dependence on a special position r, a singular point for example, we will use the notation $\mathcal{M}_r$ and $\mathcal{N}_r$ instead of $\mathcal{M}$ and $\mathcal{N}$, respectively.

The source term q in (1.1) can be any distribution function by which the solution of (1.1) is meaningful. In this paper, we will cover the general case of q containing two important cases (i) $q \in H^{-1}$, and (ii) q is a Dirac delta function, i.e. $q = \delta(\cdot - r_0)$, $r^0 \in \Omega$. It is well known that if $q \in H^{-1}$, then there is a unique weak solution $\Phi \in H^1$ satisfying (1.1) [38]. The solution Φ of (1.1) when $q = \delta(\cdot - r^0)$ is called the Robin function denoted by $R(\cdot, r_0)$. The Dirac delta function is not contained in H^{-1}, since it is contained in H^s if and only if $s < -\frac{n}{2}$ by [39]. Thus, we cannot conclude that the Robin function is contained in H^1. Rigorous definitions of the Dirac delta function and the Robin function requires use of distribution theory [40,41]. To avoid technicalities involved in distribution theory, we shall follow the concepts in [35] and use Levi functions to develop a rigorous definition of the Robin function.

The solution of (2.17a) when $q(\cdot) = \delta(\cdot - r^0)$ is called the Green, Neumann, or Robin function, depending on whether the operator $\mathcal{N}$ is Φ, $\kappa \frac{\partial \Phi}{\partial \nu}$, or (2.17b), respectively. Sometimes the Green, Neumann, and Robin functions are simply called the Green function without any regard to the boundary conditions. In this paper, however, we will use the term "Robin function".

First, we introduce the following function H which is associated with the definition of Levi functions and the Robin function.

$$H(r, r') = \begin{cases} \dfrac{1}{(n-2)\omega_n \kappa(r')} \left| r - r' \right|^{2-n} & n \ge 3, \\ \dfrac{1}{\omega_2 \kappa(r')} \log \left(\dfrac{2d}{|r - r'|} \right) & n = 2, \end{cases} \tag{2.19}$$

where $r, r' \in \mathbb{R}^n$, ω_n is the hypersurface area of the unit sphere in $\mathbb{R}^n$, and $d = \sup_{r^1, r^2 \in \Omega} |r^1 - r^2|$. The function H satisfies

$$\nabla_r \cdot (\kappa(r') \nabla_r H(r, r')) = 0 \quad \text{for } r \in \Omega \setminus \{r'\}. \tag{2.20}$$

2.1. The properties of the function H

In this subsection, the properties of the function H is presented using the Sobolev and weighted Sobolev spaces. And this properties will be used in the derivation of the Robin function in the next subsection.

Noting that $H(r', \cdot)$ has singularities only at r' with order $O(|\cdot - r'|^{2-n})$, we get the following properties of the function $H(\cdot, r')$:

$$H(\cdot, r') \in C^{\infty}(\mathbb{R}^n \setminus \{r'\}), \tag{2.21a}$$

$$H(\cdot, r') \in W^{k,p} \quad \text{if and only if } 1 \le p < \frac{n}{n+k-2}, \tag{2.21b}$$

$$H(\cdot, r') \in W^{2,\infty}_{r',2}, \quad n = 3, 4, \ldots, \tag{2.21c}$$

$$H(\cdot, r') \in W^{2,\infty}_{r',\log}, \quad n = 2, \tag{2.21d}$$

$$\frac{\partial H(\cdot, r')}{\partial r_i}, \frac{\partial H(r', \cdot)}{\partial r_i} \in W^{0,\infty}_{r',1}, \quad i = 1, \ldots, n, \tag{2.21e}$$

$$\frac{\partial^2 H(\cdot, r')}{\partial r_i \partial r_j}, \frac{\partial^2 H(r', \cdot)}{\partial r_i \partial r_j} \in W^{0,\infty}_{r',0}, \quad i, j = 1, \ldots, n. \tag{2.21f}$$

(2.21b) can be written in more detail as follows:

$$H(\cdot, r') \in L^p \quad \text{if and only if } 1 \le p < \infty \text{ when } n = 2, \tag{2.22a}$$

$$H(\cdot, r') \in W^{1,p} \quad \text{if and only if } 1 \le p < 2 \text{ when } n = 2, \tag{2.22b}$$

$$H(\cdot, r') \in L^p \quad \text{if and only if } 1 \le p < 3 \text{ when } n = 3, \tag{2.22c}$$

$$H(\cdot, r') \in W^{1,p} \quad \text{if and only if } 1 \le p < \frac{3}{2} \text{ when } n = 3, \tag{2.22d}$$

$$H(\cdot, r') \notin W^{2,p} \quad \text{for } n = 2, 3, \ldots. \tag{2.22e}$$

(2.21c)–(2.21f) is proved by the following computations:

$$\|H(\cdot, r)\|_{W^{0,\infty}_{r,2}}, \|H(r, \cdot)\|_{W^{0,\infty}_{r,2}} \le \frac{1}{\max(1, n-2)\omega_n L}, \tag{2.23a}$$

$$\left\| \frac{\partial H(\cdot, r')}{\partial r_i} \right\|_{W^{0,\infty}_{r',1}} \le \frac{1}{\omega_n L}, \tag{2.23b}$$

$$\left\| \frac{\partial^2 H(\cdot, r')}{\partial r_i \partial r_j} \right\|_{W^{0,\infty}_{r',0}} \le \frac{n}{\omega_n L}, \tag{2.23c}$$

for all $i, j = 1, \ldots, n$. For (2.23a), the assumption (1.2) is used. If $L < |\frac{\partial \kappa(r)}{\partial r_i}| < U$ is assumed along with (1.2), then

$$\left\| \frac{\partial H(r', \cdot)}{\partial r_i} \right\|_{W^{0,\infty}_{r',1}} \le \left(1 + \frac{U}{\max(1, n-2)L}\right) \frac{1}{\omega_n L}, \tag{2.24}$$

and further, if $L < |\frac{\partial^2 \kappa(r)}{\partial r_i \partial r_j}| < U$ is assumed along with the above conditions, then

$$\left\| \frac{\partial^2 H(r', \cdot)}{\partial r_i \partial r_j} \right\|_{W^{0,\infty}_{r',0}} \le \left(n + \frac{2U}{L} + \frac{3U^2}{L^2}\right) \frac{n}{\omega_n L}. \tag{2.25}$$

2.2. Levi function and Robin function

In this subsection, we provide precise definitions of the Robin function and investigate the properties of the Robin function. To do that, the definitions and properties of the Levi function will be introduced following the approaches in [35].

Definition 2.1 (*Levi Function*)**.** A function $L(r, r')$, $r, r' \in \Omega$ is called a *Levi function* if $L(\cdot, r') \in C^2(\Omega \setminus \{r'\})$, and $L(\cdot, r') - H(\cdot, r') \in W^{2,\infty}_{r',2+\lambda}$ for some constant $\lambda > 0$, where λ is the order of the Levi function.

Note that $H(r, r')$ is a Levi function and $H(r', r)$ is also a Levi function of order 1 if $\kappa \in W^{2,\infty}$. Thus, if $L(r, r')$ is a Levi function of order λ, then $L(r', r)$ a Levi function of order $\min(\lambda, 1)$. Before introducing the properties of the Levi function in the following lemmas, let us state some known results.

Let $K(r, \cdot) \in W^{0,\infty}_{r,\alpha}$, $\alpha > 0$ and

$$u(r) = \int_\Omega K(r, r')\phi(r')\mathrm{d}r'. \tag{2.26}$$

If K is a Levi function, then $\alpha \le 2$ for $n \ge 3$ and $\alpha < 2$ for $n = 2$, and if K is a derivative of a Levi function, $\alpha \le 1$. However, if K is a second derivative of a Levi function, we must choose $\alpha \le 0$ and hence cannot use (2.27).

Then the following facts are known [17]:

- There exists a constant $C_1 = C_1(\alpha, p, q)$ such that:

$$\|u\|_{L^q} \le C_1(\alpha, p, q) \sup_{r\in\Omega} \|K(r, \cdot)\|_{W^{0,\infty}_{r,\alpha}} \|\phi\|_{L^p} \quad \text{for } 0 < \alpha < \frac{n}{p} \le \alpha + \frac{n}{q}. \tag{2.27}$$

- The maximum value of q in (2.27) is taken as follows :

$$\|u\|_{L^{\frac{np}{n-\alpha p}}} \le C_1(\alpha, p) \sup_{r\in\Omega} \|K(r, \cdot)\|_{W^{0,\infty}_{r,\alpha}} \|\phi\|_{L^p} \quad \text{for } p < \frac{n}{\alpha}, \tag{2.28a}$$

$$\|u\|_{L^{\frac{n}{\epsilon}}} \le \widetilde{C}_1(\epsilon) d^\epsilon \sup_{r\in\Omega} \|K(r, \cdot)\|_{W^{0,\infty}_{r,\alpha-\epsilon}} \|\phi\|_{L^p} \quad \text{for } p = \frac{n}{\alpha}, \tag{2.28b}$$

  where ϵ is some constant between 0 and α, $C_1(\alpha, p) = C_1\left(\alpha, p, \frac{np}{n-\alpha p}\right)$, and $\widetilde{C}_1(\epsilon) = C_1(\alpha - \epsilon, \frac{n}{\alpha}, \frac{n}{\epsilon})$.
- We also have the following inequality:

$$\|u\|_{C^0} \le C_2(p) \sup_{r\in\Omega} \|K(r, \cdot)\|_{W^{0,\infty}_{r,\alpha}} \|\phi\|_{L^p}, \quad \text{for } p > \frac{n}{\alpha}, \tag{2.29}$$

  where $C_2(p)$ is a constant depending on p.
- When $K = \frac{\partial^2 H}{\partial r_i \partial r_j}$, there exists a constant C_3 [16] such that:

$$\|u\|_{L^p} \le \frac{C_3}{L} \|\phi\|_{L^p}. \tag{2.30}$$

By summing up the results (2.27)–(2.29), the integral operator defined in (2.26) is a bounded linear operator from $W^{1,p}$ into $W^{1,p}$.

Although the constants in this paper may depend on n, we will neglect this dependence on n unless it is needed. Using (2.27) and (2.30), we obtain the following lemma about the properties of the Levi function.

Lemma 2.2. *Let $L(\cdot, r')$ be a Levi function of order $\lambda > 0$ and assume $\kappa \in C^{0,\lambda}$ and $\partial\Omega \in C^{1,\lambda}$. Let $\psi \in L^p$, where $p \ge 1$ and define v as*

$$v(r) = \int_\Omega L(r, r')\psi(r')\mathrm{d}r'. \tag{2.31}$$

Then, $\frac{\partial v}{\partial r_i}$, where $i = 1, \ldots, n$ are absolutely continuous on one-dimensional line parallel to the r_i-axis, $\frac{\partial^2 v}{\partial r_i \partial r_j} \in L^p$, $i, j = 1, \ldots, n$, and the following bounds hold:

$$\|v\|_{L^p} \le C_1\left(\min\left(\frac{n}{p}, 2\right), p, p\right) \sup_{r\in\Omega} \|L(r, \cdot)\|_{W^{0,\infty}_{r,2}} \|\psi\|_{L^p} \quad n \ge 3, \tag{2.32a}$$

$$\|v\|_{L^p} \le C_1\left(\min\left(\frac{2}{p}, 2\right) - \epsilon, p, p\right) \sup_{r\in\Omega} \|L(r, \cdot)\|_{W^{0,\infty}_{r,2}} \|\psi\|_{L^p} \quad n = 2, 0 < \epsilon < 2, \tag{2.32b}$$

$$\left\|\frac{\partial v}{\partial r_i}\right\|_{L^p} \le C_1\left(\min\left(\frac{n}{p}, 1\right), p, p\right) \sup_{r'\in\Omega} \left\|\frac{\partial L(r', \cdot)}{\partial r_i}\right\|_{W^{0,\infty}_{r',2}} \|\psi\|_{L^p} \quad i = 1, \ldots, n, \tag{2.32c}$$

$$\left\|\frac{\partial^2 v}{\partial r_i \partial r_j}\right\|_{L^p} \le \left[C_1(\lambda, p, p) \sup_{r'\in\Omega} \left\|\frac{\partial^2 (L - H)(r', \cdot)}{\partial r_i \partial r_j}\right\| + \frac{C_3}{L} + \frac{1}{nL}\right] \|\psi\|_{L^p} \quad i, j = 1, \ldots, n, \tag{2.32d}$$

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where C_1 and C_2 are introduced in (2.27) and (2.29), respectively. Furthermore, the following equations hold:

$$\frac{\partial v}{\partial r_i}(\mathrm{r}) = \int_\Omega \frac{\partial L}{\partial r_i}(\mathrm{r},\mathrm{r}')\psi(\mathrm{r}')\mathrm{dr}', \tag{2.33a}$$

$$\frac{\partial^2 v}{\partial r_i \partial r_j}(\mathrm{r}) = -\frac{1}{n\kappa(\mathrm{r})}\psi(\mathrm{r}) + \lim_{\epsilon\to 0}\int_{\Omega\setminus\overline{B(x,\epsilon)}} \frac{\partial^2 L}{\partial r_i\partial r_j}(\mathrm{r},\mathrm{r}')\psi(\mathrm{r}')\mathrm{dr}', \tag{2.33b}$$

$$\mathcal{M}_r v(\mathrm{r}) = -\psi(\mathrm{r}) + \int_\Omega \mathcal{M}_r L(\mathrm{r},\mathrm{r}')\psi(\mathrm{r}')\mathrm{dr}'. \tag{2.33c}$$

If $v \in W^{2,p}$, then

$$v(\mathrm{r}) = \int_\Omega v(\mathrm{r}')\mathcal{M}_{r'}L(\mathrm{r},\mathrm{r}') - \mathcal{M}v(\mathrm{r}')L(\mathrm{r},\mathrm{r}')\mathrm{dr}' + \int_{\partial\Omega}(\mathcal{N}v(\mathrm{r}')L(\mathrm{r},\mathrm{r}') - v(\mathrm{r}')\mathcal{N}_r L(\mathrm{r},\mathrm{r}'))\mathrm{d}S(\mathrm{r}'). \tag{2.34}$$

Proof. See Appendix A. □

Definition 2.3 (*Robin Function*)**.** A Levi function R of order $\lambda > 0$, which is a solution of the equations

$$\mathcal{M}_r R(\mathrm{r},\mathrm{r}') = 0 \quad \text{for } \mathrm{r} \in \Omega \setminus \{\mathrm{r}'\}, \tag{2.35a}$$

$$\mathcal{N}_r R(\mathrm{r},\mathrm{r}') = 0 \quad \text{for } \mathrm{r} \in \partial\Omega \setminus \{\mathrm{r}'\}, \tag{2.35b}$$

is called a Robin function. Note that $\mathcal{M}_r$ and $\mathcal{N}_r$ are the complex conjugate operators for $\mathcal{M}_r$ and $\mathcal{N}_r$, respectively.

A few existence theorems of Robin functions can be found in Section 19 and Section 22 in [35]. For the rest of the paper, we assumed that the Robin function exists for Ω, κ, and μ_a. Note that if the Robin function exists, it is unique. A Levi function which satisfies (2.35a) but not necessarily (2.35b) is called a fundamental solution. If $\kappa \in C^{2,\lambda}$ and $\mu_a \in C^{0,\lambda}$, there exists a fundamental solution for $\mathcal{M}$ in Ω by Theorem 19.VIII and Section 22 in [35]. However, even though fundamental solutions exists, these solutions are not unique. For example, H is a fundamental solution for (1.1) when $\mu_a = 0$, $\omega = 0$, and $\delta\kappa = 0$.

The properties of the Robin function is presented in the next Lemma 2.4.

Lemma 2.4. *Let $R(\cdot, \mathrm{r}')$ be a Robin function of order $\lambda > 0$, $\kappa \in C^{0,\lambda}$, and $\partial\Omega \in C^{1,\lambda}$. Let $\psi \in L^p$, where $p \geq 1$ and v be given by*

$$v(\mathrm{r}) = \int_\Omega R(\mathrm{r},\mathrm{r}')\psi(\mathrm{r}')\mathrm{dr}'. \tag{2.36}$$

Then (2.32)–(2.34) hold, replacing the Levi function L with the Robin function R. Furthermore, we get the following equations for v with the Robin function as the kernel:

$$\mathcal{M}_r v(\mathrm{r}) = -\psi(\mathrm{r}), \tag{2.37a}$$

$$v(\mathrm{r}) = -\int_\Omega R(\mathrm{r},\mathrm{r}')\mathcal{M}v(\mathrm{r}')\mathrm{dr}' + \int_{\partial\Omega} R(\mathrm{r},\mathrm{r}')\mathcal{N}v(\mathrm{r}')\mathrm{d}S(\mathrm{r}'), \quad \textit{if } v \in W^{2,p}, \tag{2.37b}$$

$$v(\mathrm{r}) = \int_\Omega R(\mathrm{r},\mathrm{r}')q(\mathrm{r}')\mathrm{dr}', \quad \textit{if } v \textit{ satisfies } (2.18) \textit{ and } q \in L^p, \tag{2.37c}$$

$$R(\mathrm{r},\mathrm{r}') = \overline{R}(\mathrm{r}',\mathrm{r}). \tag{2.37d}$$

Proof. (2.32), (2.33), and (2.34) hold because a Robin function is also a Levi function. (2.37a) is derived by using the definition of the Robin function and (2.33c). Using (2.34), we derive (2.37b) and (2.37c). (2.37d) is induced from the fact that the adjoint operator of $\mathcal{M}$ is the complex conjugate of $\mathcal{M}$ and Theorem 10.I in [35]. □

3. Born expansion

In this section, we define Born expansion in the normed spaces introduced in Section 2.1, and discuss the validity of Born expansion and compute the error between the infinite order Born expansion and the finite order Born approximation using the inequalities developed in Section 2.2. In Section 3.1, we will analyze the Born expansion when both the absorption(μ_a) and the diffusion(κ) coefficients are perturbed. In Section 3.2., we analyzed the Born expansion when the diffusion coefficient is fixed and only the absorption coefficient is perturbed.

Note that in the derivation of (1.12), (2.37c) was used. Thus (1.12) holds when $\widetilde{\Phi} \in L^p$, since $H^1 \subset L^2$ and the Robin function is contained in L^p for all $p \geq 1$, $(n = 2)$ and $1 \leq p < \frac{n}{n-2}$, $(n \geq 3)$. (1.12) holds at least for the Robin function and the H^1 functions.

The formal expansion (1.13) exists only if $\mathcal{R}^k\Phi$, where $k = 1, \dots, m$ is defined. We provide the following definition related to the definition of $\mathcal{R}^k\Phi$, where $k = 1, \dots, m$.

Definition 3.1 (*mth Order Representation, Infinite Order Representation with Index M*)**.** The integral operator $\mathcal{R}$ is called to have an mth order representation

$$B_0 \to B_1 \to B_2 \to B_3 \to \cdots \to B_m. \tag{3.38}$$

if there are normed spaces B_k, where $k = 0, 1, \dots, m$ such that $\mathcal{R}(B_{k-1}) \subset B_k$ for all $k = 1, \dots, m$. And the operator $\mathcal{R}$ is called to have an infinite order representation with an index M

$$B_0 \to B_1 \to B_2 \to B_3 \to \cdots \to B_M \to B_M \to \cdots, \tag{3.39}$$

if there are $M + 1$ normed spaces $B_0, B_1, \dots, B_M$ such that $\mathcal{R}(B_{k-1}) \subset B_k$ for all $k = 1, \dots, M$.

If $\mathcal{R}$ has mth order representation, we define $E^m\Phi$ and $F^m\Phi$ as follows:

$$E^m\Phi = \Phi + \mathcal{R}\Phi + \mathcal{R}^2\Phi + \cdots + \mathcal{R}^{m-1}\Phi + \mathcal{R}^m\widetilde{\Phi}, \tag{3.40a}$$

$$F^m\Phi = \Phi + \mathcal{R}\Phi + \mathcal{R}^2\Phi + \cdots + \mathcal{R}^{m-1}\Phi + \mathcal{R}^m\Phi. \tag{3.40b}$$

If the operator $\mathcal{R}$ has mth order representation, then

$$E^1 = E^2 = \cdots = E^m, \qquad E^m\Phi = \widetilde{\Phi}. \tag{3.41}$$

by (1.13). If $\mathcal{R}$ has infinite order representation with an index M, then (3.41) holds for all $m \geq 1$. If we define $E^\infty\Phi$ as

$$E^\infty\Phi = \Phi^{(0)} + \Phi^{(1)} + \Phi^{(2)} + \cdots + \Phi^{(m-1)} + \Phi^{(m)} + \cdots, \tag{3.42}$$

then $E^\infty\Phi \in B_M$ and we can easily show that

$$E^\infty = E^1 = \cdots = E^m = \cdots, E^\infty\Phi = \widetilde{\Phi}. \tag{3.43}$$

Further3.2more, if the operator $\mathcal{R}$ has an infinite order representation, we have the following proposition:

Proposition 3.2. *Assume that the operator $\mathcal{R}$ has an infinite order representation with an index M. If $\{F^m\Phi\}_{m=M,M+1,\dots}$ converges, the limit is $E^\infty\Phi \in B_M$. The necessary and sufficient condition for $F^m\Phi$, $m = M, M+1, \dots$ to converge to $E^\infty\Phi$ is*

$$\lim_{k\to\infty} \left\| \mathcal{R}^{M+k}\widetilde{\Phi} \right\|_{B_M} = 0. \tag{3.44}$$

The sufficient condition for (3.44) is

$$\|\mathcal{R}\|_{B_M\to B_M} < 1. \tag{3.45}$$

Proof. Since $E^\infty\Phi - F^m\Phi = E^{m+1}\Phi - F^m\Phi = \mathcal{R}^{m+1}\widetilde{\Phi}$, (3.44) is the necessary and sufficient condition for $F^m\Phi$ to converge to $E^\infty\Phi$. If $\|\mathcal{R}\|_{B_M\to B_M} < 1$, then

$$\begin{aligned} \left\| \mathcal{R}^{M+k}\Phi \right\|_{B_M} &\leq \left\| \mathcal{R}^k \right\|_{B_M\to B_M} \left\| \mathcal{R}^M\Phi \right\|_{B_M} \\ &\leq \|\mathcal{R}\|^k_{B_M\to B_M} \left\| \mathcal{R}^M\Phi \right\|_{B_M} \to 0 \text{ as } k \to \infty. \quad \square \end{aligned} \tag{3.46}$$

Definition 3.3 (*mth Order Born Approximation, (mth Order, Infinite Order) Born Expansion*)**.** If $\mathcal{R}$ has an mth order representation, $E^m\Phi$ and $F^m\Phi$ defined in (3.40) are called the mth order Born approximation and mth order Born expansion, respectively. If $\mathcal{R}$ has an infinite order representation, $E^\infty\Phi$ defined in (3.42) is an infinite order Born expansion. Since $E^m\Phi = E^\infty\Phi$, $m \geq 1$ by (3.43), E^∞ and E^m are just called Born expansion without any discrimination of orders.

Using Proposition 3.2, we investigate the following three questions about Born expansion and Born approximation, which corresponds to the questions raised in the introduction:

- When does the infinite order Born expansion E^∞ exist? In other words, is there an infinite order representation with an index M for the operator $\mathcal{R}$ such that

$$B_0 \to B_1 \to B_2 \to B_3 \to \cdots \to B_M \to B_M \to \cdots, \tag{3.47}$$

as in (3.39).
- Assume that there exists an infinite order representation with an index M (3.47) for the operator $\mathcal{R}$. By Proposition 3.2, (3.44) and (3.45) are the equivalent condition and the sufficient condition, respectively, for the Born approximations F^m converge to the Born expansion E^∞. Then, what are the conditions on $\delta\mu$ for the operator $\mathcal{R}$ to satisfy (3.45)?

- Assume that F^m converges to E^∞. Then, what is the error between F^m and E^∞? In other words, what is the norm bound of $\widetilde{\Phi}^{(m+1)} = E^\infty - F^m$?

Although it is possible to compute the error of the Born approximation when E^∞ does not exist or F^m does not converge to E^∞, we will only treat the case when E^∞ exists and F^m converges to E^∞. In the following subsections, we first relate $\mathcal{R}$ with infinite order representation, then we argue about the condition on the optical coefficients for the norm of $\mathcal{R}$ to be less than 1. Finally, we compute the error in the mth order Born approximation and the Born expansion.

3.1. The Born expansion when both the diffusion and absorption coefficients are perturbed

In this subsection, we treat the Born expansion when both the diffusion and absorption coefficients are perturbed. By Proposition 3.2, we need to define the operator $\mathcal{R}$ recursively to define Born expansion, which requires the behavior of $\nabla\mathcal{R}$ near the singular point. The kernel of the integral operator $\nabla\mathcal{R}_1$ is the derivative of Robin function, which is a weakly singular kernel contained in $W^{0,\infty}_{r_0,1}$. However, the kernel of $\nabla\mathcal{R}_2$ is the second derivative of the Robin function, which is classified to hyper singular kernel and the inter integral operator with hyper singular kernel is not necessarily integrable. Note that the treatment of the integral operator with hyper singular kernels is more difficult as compared to the treatment of the integral operator with weak singular kernels [42].

To do a quantitative analysis, let us define the following bounds for the Robin function:

$$S(n) := \sup_{r\in\Omega} \|R(r,\cdot)\|_{W^{1,\infty}_{r,2}}, \quad n \geq 3, \tag{3.48a}$$

$$S(n) := \sup_{r\in\Omega} \|R(r,\cdot)\|_{W^{1,\infty}_{r,\log}}, \quad n = 2, \tag{3.48b}$$

$$T(n) := \sup_{r\in\Omega} \|(R-H)(r,\cdot)\|_{W^{2,\infty}_{r,2}}. \tag{3.48c}$$

Lemma 3.4. *$\mathcal{R}_1$ and $\mathcal{R}_2$ are bounded with respect to the $W^{1,p}$ norm:*

$$\|\mathcal{R}_1\|_{W^{1,p}\to W^{1,p}} \leq C_4 \|\delta\mu_a\|_{L^\infty}, \tag{3.49a}$$

$$\|\mathcal{R}_2\|_{W^{1,p}\to W^{1,p}} \leq C_5 \|\delta\kappa\|_{L^\infty}, \tag{3.49b}$$

where

$$C_4 = S(n) \max\left(C_1\left(\min\left(\frac{n}{p},2\right),p,p\right), C_1\left(\min\left(\frac{n}{p},1\right),p,p\right)\right), \quad n \geq 3, \tag{3.50a}$$

$$C_4 = S(n) \max\left(C_1(2-\epsilon,p,p), C_1\left(\min\left(\frac{2}{p},1\right),p,p\right)\right), \quad n = 2, 0<\epsilon<2, \tag{3.50b}$$

$$C_5 = C_1(\min\left(\frac{n}{p},1\right),p,p)S(n) + C_1(\lambda,p,p)T(n) \quad + \frac{C_3 n^2}{L} + \frac{n}{L}. \tag{3.50c}$$

Proof. Let $\psi \in W^{1,p}$, then by (2.32a)–(2.32c),

$$\left\|\int_\Omega R(r,r')\delta\mu_a(r')\psi(r')\mathrm{d}r'\right\|_{L^p} \leq C_1(\min(n/p,2),p,p)\,\|R(r,\cdot)\|_{L^p}\,\|\delta\mu_a\|_{L^\infty}\,\|\psi\|_{L^p}, \quad n\geq 3, \tag{3.51a}$$

$$\left\|\int_\Omega R(r,r')\delta\mu_a(r')\psi(r')\mathrm{d}r'\right\|_{L^p} \leq C_1(2/p-\epsilon,p,p)\,\|R(r,\cdot)\|_{L^p}\,\|\delta\mu_a\|_{L^\infty}\,\|\psi\|_{L^p}, \quad n=2, 0<\epsilon<2, \tag{3.51b}$$

$$\left\|\int_\Omega \frac{\partial R(r,r')}{\partial r_i}\delta\mu_a(r')\psi(r')\mathrm{d}r'\right\|_{L^p} \leq C_1(\min(n/p,1),p,p)\left\|\frac{\partial R(r,\cdot)}{\partial r_i}\right\|_{L^p}\|\delta\mu_a\|_{L^\infty}\,\|\psi\|_{L^p}, \quad i=1,\ldots,n. \tag{3.51c}$$

(3.49a) is derived from (3.51) by defining C_4 as in (3.50a) and (3.50b). Using (2.32c), (2.32d), and (2.37d), we obtain

$$\left\|\int_\Omega \frac{\partial R(r,r')}{\partial r'_i}\delta\kappa(r')\frac{\partial\psi(r')}{\partial r'_i}\mathrm{d}r'\right\|_{L^p} = \left\|\int_\Omega \frac{\partial\overline{R}(r',r)}{\partial r'_i}\delta\kappa(r')\frac{\partial\psi(r')}{\partial r'_i}\mathrm{d}r'\right\|_{L^p}$$

$$\leq C_1(\min(n/p,1),p,p)\left\|\frac{\partial R(r,\cdot)}{\partial r_i}\right\|_{L^p}\|\delta\kappa\|_{L^\infty}\,\|\psi\|_{W^{1,p}}, \quad n\geq 3, i=1,\ldots,n, \tag{3.52a}$$

$$\left\|\int_\Omega \frac{\partial R(r,r')}{\partial r'_i}\delta\kappa(r')\frac{\partial\psi(r')}{\partial r'_i}\mathrm{d}r'\right\|_{L^p}$$

$$\leq C_1(2/p-\epsilon,p,p)\,\|R(r,\cdot)\|_{L^p}\,\|\delta\kappa\|_{L^\infty}\,\|\psi\|_{W^{1,p}}, \quad n=2, 0<\epsilon<2, i=1,2, \tag{3.52b}$$

$$\left\| \int_{\Omega} \frac{\partial^2 R(r, r')}{\partial r_i' \partial r_j'} \delta\kappa(r')\psi(r')\mathrm{d}r' \right\|_{L^p} = \left\| \int_{\Omega} \frac{\partial^2 R(r, r')}{\partial r_i \partial r_j} \delta\kappa(r')\psi(r')\mathrm{d}r' \right\|_{L^p}$$

$$\leq \|\delta\kappa\|_{L^\infty} \|\psi\|_{W^{1,p}} \cdot \left(C_1 \left(\min\left(\frac{n}{p}, 1\right), p, p \right) S(n) + C_1(\lambda, p, p)T(n) + \frac{C_3 n^2}{L} + \frac{n}{L} \right). \tag{3.52c}$$

Using (3.52) and defining C_5 as in (3.50c), we obtain (3.49b). □

Using Lemma 3.4, we state and prove the following results about Born expansion and Born approximation when both the absorption and reduced scattering coefficients are perturbed.

Theorem 3.5. *The integral operator $\mathcal{R}$ has an infinite order representation with the index $M = 1$ as follows:*

$$W^{1,p} \to W^{1,p} \to W^{1,p} \to \cdots. \tag{3.53}$$

If

$$C_4 \|\delta\mu_a\|_\infty + C_5 \|\delta\kappa\|_\infty < 1 \tag{3.54}$$

holds, then $E^\infty \Phi$ exists for the representation given in (3.53) and the mth order Born approximation $F^m\Phi$ converges to $E^\infty\Phi$ for $\Phi \in W^{1,p}$. Furthermore, the error between $\widetilde{\Phi} = E^\infty\Phi$ and $F^{m-1}\Phi$ is given as follows:

$$\left\|\widetilde{\Phi} - F^m\Phi\right\|_{W^{1,p}} \leq (C_4 \|\delta\mu_a\|_\infty + C_5 \|\delta\kappa\|_\infty)^m \left\|\widetilde{\Phi}\right\|_{W^{1,p}}. \tag{3.55}$$

Proof. From (3.49), we can derive

$$\|\mathcal{R}\|_{W^{1,p}\to W^{1,p}} \leq C_4 \|\delta\mu_a\|_{L^\infty} + C_5 \|\delta\kappa\|_{L^\infty}. \tag{3.56}$$

Hence (3.53) holds, and (3.54) is the sufficient condition for the existence of E^∞ by Proposition 4.2. (3.55) holds using (3.56) and the following inequality:

$$\widetilde{\Phi} - F^{m-1}\Phi = \widetilde{\Phi}^{(m)} = \mathcal{R}^m\Phi. \quad \square \tag{3.57}$$

3.2. Born expansion when only the absorption coefficient is perturbed

In this subsection, we will study the Born expansion and the Born approximation when $\delta\kappa = 0$ and $\delta\mu_a \neq 0$. Since $\mathcal{R} = \mathcal{R}_1$ due to $\delta\kappa = 0$, we do not need to treat the second or first derivatives of the Robin function as the kernel of the integral operator $\mathcal{R}$. That is to say, we do not need to handle integral operators with hyper singular kernel.

Before analyzing the Born expansion in the normed spaces in L^p, where $p \geq 1$, L^∞, $W^{0,\infty}_{r_0,\log}V(n = 2)$, and $W^{0,\infty}_{r_0,2}(n \geq 3)$ for $r_0 \in \Omega$, we first state some inequalities:

Lemma 3.6. *Let $0 < \alpha_1, \alpha_2 < n$ and $r^1, r^2 \in \Omega$, then*

$$\text{(i)} \quad \int_\Omega \log(2d/|r^1 - r'|)\mathrm{d}r' \leq (\log(2) + 1)\omega_2 d, \quad n = 2, \tag{3.58a}$$

$$\text{(ii)} \quad \int_\Omega |r^1 - r'|^{\alpha_1 - n}\mathrm{d}r' \leq \omega_n \frac{d^{\alpha_1}}{\alpha_1}, \tag{3.58b}$$

$$\text{(iii)} \quad \int_\Omega \log(2d/|r^1 - r'|)\log(2d/|r^2 - r'|)\mathrm{d}r' \leq C_6\omega_2 d^2, \quad n = 2, \tag{3.58c}$$

$$\text{(iv)} \quad \int_\Omega |r^1 - r'|^{\alpha_1 - n}|r' - r^2|^{\alpha_2 - n}\mathrm{d}r', \leq C_7(\alpha_1, \alpha_2)\omega_n |r^1 - r^2|^{\alpha_1 + \alpha_2 - n} \quad \textit{if } \alpha_1 + \alpha_2 < n, \tag{3.58d}$$

$$\leq C_8(\alpha_1, \alpha_2)\omega_n \log(2d/|r^1 - r^2|) \quad \textit{if } \alpha_1 + \alpha_2 = n, \tag{3.58e}$$

$$\leq C_7(\alpha_1, \alpha_2)\omega_n d^{\alpha_1 + \alpha_2 - n} \quad \textit{if } \alpha_1 + \alpha_2 > n, \tag{3.58f}$$

$$\text{(v)} \quad \int_\Omega |r^1 - r'|^{\alpha_1 - n}\log(2d/|r' - r^2|)\mathrm{d}r' \leq C_9(\alpha_1)\omega_n d^{\alpha_1}, \tag{3.58g}$$

where

$$C_6 \leq \frac{1}{4}(6(\log 2)^2 + 2\log 2\log 3 + \log 3 - \log 2 - 1) < 1,$$

$$C_7(\alpha_1, \alpha_2) = 2^{n - \alpha_1 - \alpha_2}\left[\frac{3^{n - \max(\alpha_1, \alpha_2)}}{n - \alpha_1 - \alpha_2} + \frac{1}{\alpha_1} + \frac{1}{\alpha_2}\right],$$

$$C_8(\alpha_1,\alpha_2) = \left[3^{n-\max(\alpha_1,\alpha_2)} + \frac{1}{\alpha_1 \log 2} + \frac{1}{\alpha_2 \log 2}\right],$$
$$C_9(\alpha_1) = \frac{\log 4}{\alpha_1 2^{\alpha_1}} + \frac{\log 4 + \frac{1}{n}}{n 2^{\alpha_1}} + \frac{\log 6 + \frac{1}{\alpha_1}}{\alpha_1}.$$

Proof. See Appendix B. □

To do a quantitative analysis, let us define the following bounds for the Robin function

$$U(n) := \sup_{r\in\Omega} \|R(r,\cdot)\|_{W^{0,\infty}_{r,2}}, \quad n \ge 3, \tag{3.59a}$$
$$U(n) := \sup_{r\in\Omega} \|R(r,\cdot)\|_{W^{0,\infty}_{r,\log}}, \quad n = 2, \tag{3.59b}$$
$$U(n,\epsilon) := \sup_{r\in\Omega} \|R(r,\cdot)\|_{W^{0,\infty}_{r,2-\epsilon}}, \quad n \ge 3, 0 < \epsilon < 2. \tag{3.59c}$$

With the aid of Lemma 3.6, we are able to state and prove the following inequalities for the integral operator $\mathcal{R}_1$.

Lemma 3.7. *We have the following norm bounds for the integral operator* $\mathcal{R}_1$*:*

$$\text{(i) } \|\mathcal{R}_1\|_{L^p\to L^p} \le C_1\left(\min\left(\frac{n}{p},2\right),p,p\right) U(n)\,\|\delta\mu_a\|_{L^\infty}, \quad n \ge 3, \tag{3.60a}$$
$$\text{(ii) } \|\mathcal{R}_1\|_{L^p\to L^p} \le C_1\left(\frac{2}{p}-\epsilon,p,p\right) U(n)\,\|\delta\mu_a\|_{L^\infty}, \quad n = 2, 0<\epsilon<2, \tag{3.60b}$$
$$\text{(iii) } \|\mathcal{R}_1\|_{L^\infty\to L^\infty} \le C_{10}\omega_n U(n)\,\|\delta\mu_a\|_{L^\infty}, \tag{3.60c}$$
$$\text{(iv) } \|\mathcal{R}_1\|_{W^{0,\infty}_{r,2}\to W^{0,\infty}_{r,2}} \le C_7(2,2)\omega_n U(n)\,\|\delta\mu_a\|_\infty \quad n = 3,5,6,\ldots, \tag{3.60d}$$
$$\text{(v) } \|\mathcal{R}_1\|_{W^{0,\infty}_{r,2}\to W^{0,\infty}_{r,2}} \le C_8(2,2)\omega_4 U(4)\,\|\delta\mu_a\|_\infty \quad n = 4, \tag{3.60e}$$
$$\text{(vi) } \|\mathcal{R}_1\|_{W^{0,\infty}_{r,\log}\to W^{0,\infty}_{r,\log}} \le C_6 \log 2\omega_2 U(2)\,\|\delta\mu_a\|_\infty \quad n = 2, \tag{3.60f}$$

where the constant C_{10} *is given by*

$$C_{10} = (\log 2 + 1)d, \quad n = 2, \tag{3.61a}$$
$$C_{10} = \frac{d^2}{2}, \quad n \ge 3. \tag{3.61b}$$

Proof. (3.60a) and (3.60c) result from (2.32a) and (2.32b), respectively. (3.60c) is derived from (3.58a) for two dimensions, and (3.58b) for n dimensions ($n \ge 3$) with $\alpha_1 = 2$. (3.60d) is obtained from (3.58d), (3.58f), and by using $|r_1 - r_2| \le d$ for all $r_1, r_2 \in \Omega$. Similarly, (3.60e) and (3.60d) are derived from (3.58e) and (3.58g), respectively. □

By using Lemma 3.7, we give the following theorem about Born expansion and Born approximation :

Theorem 3.8. *The integral operator* $\mathcal{R} = \mathcal{R}_1$ *has the following infinite order representation with an index* $M = 1$ *such that*

$$L^p \to L^p \to L^p \to L^p \to \cdots, \quad p \ge 1, \tag{3.62a}$$
$$L^\infty \to L^\infty \to L^\infty \to L^\infty \to \cdots, \tag{3.62b}$$
$$W^{0,\infty}_{r,2} \to W^{0,\infty}_{r,2} \to W^{0,\infty}_{r,2} \to \cdots, \quad n \ge 3, \tag{3.62c}$$
$$W^{0,\infty}_{r,\log} \to W^{0,\infty}_{r,\log} \to W^{0,\infty}_{r,\log} \to W^{0,\infty}_{r,\log} \to \cdots \quad n = 2. \tag{3.62d}$$

Let us define a constant $C_{11} = C_{11}(B)$ *depending on the normed space* $B = L^p (p \ge 1), L^\infty, W^{0,\infty}_{r,2}$*, or* $W^{0,\infty}_{r,\log}$ *as follows:*

$$C_{11} = C_{11}(B) = \begin{cases} C_1\left(\min\left(\frac{n}{p},2\right),p,p\right)U(n), & \text{if } B = L^p \text{ and } n \ge 3,\\ C_1\left(\frac{2}{p}-\epsilon,p,p\right)U(2), & \text{if } B = L^p, n = 2,\\ C_{10}\omega_n U(n), & \text{if } B = L^\infty,\\ C_7(2,2)\omega_n U(n), & \text{if } B = W^{0,\infty}_{r,2} \text{ and } n = 3,5,6,\ldots,\\ C_8(2,2)\omega_4 U(4), & \text{if } B = W^{0,\infty}_{r,2} \text{ and } n = 4,\\ C_6 \log 2\omega_2 U(2), & \text{if } B = W^{0,\infty}_{r,\log} \text{ and } n = 2, \end{cases}$$

where $0 < \epsilon < 2$ and $r \in \Omega$. If the following condition

$$\|\delta\mu_a\|_\infty < \frac{1}{C_{11}(B)} \tag{3.63}$$

holds, then $E^\infty\Phi$ exists for each representation given in (3.62) and the mth order Born approximation $F^m\Phi$ converges to $E^\infty\Phi$ for $\Phi \in B$. Furthermore, the error between $\widetilde{\Phi} = E^\infty\Phi$ and $F^{m-1}\Phi$ is given by:

$$\left\|\widetilde{\Phi} - F^{m-1}\Phi\right\|_B \le \left(C_{11}(B)\,\|\delta\mu_a\|_\infty\right)^m \left\|\widetilde{\Phi}\right\|_B . \tag{3.64}$$

The proof of Theorem 3.8 is obtained by Proposition 3.2 and Lemma 3.7, which is similar to the proof of Theorem 3.5. In Theorems 3.5 and 3.8, the same normed space is used for the infinite order representations with indices $M = 1$. However, the following theorem is another kind of infinite order representation for the operator $\mathcal{R}$ with an index $M \neq 1$.

Theorem 3.9. *The operator $\mathcal{R}$ has the following infinite order representations with indices $M \ge 2$ and $B_M = C^0$, where C^0 is the normed space of continuous functions having the norm $\|\cdot\|_{L^\infty}$:*

$$L^\infty \to C^0 \to C^0 \to C^0 \to C^0 \to C^0 \to \cdots, \quad \text{for } n = 2, 3, 4, \ldots, \tag{3.65a}$$

$$L^{\frac{n}{2k}} \to L^{\frac{n}{2(k-1)}} \to \cdots \to L^{n/2} \to L^{\frac{n}{\epsilon}} \to C^0 \to C^0 \to \cdots, \quad \text{for } 1 \le p = \frac{n}{2k} \text{ and } k \text{ is a positive integer}, \tag{3.65b}$$

$$L^p \to L^{\frac{np}{n-2p}} \to \cdots \to L^{\frac{np}{n-2lp}} \to C^0 \to C^0 \to \cdots,$$
$$\text{for } l = \left[\frac{n-2p}{2p}\right] \ge 0,\ 1 \le p \ne \frac{n}{2k}, \quad \text{and } k \text{ is a positive integer}, \tag{3.65c}$$

$$W^{0,\infty}_{r_0,2} \to W^{0,\infty}_{r_0,4} \to \cdots \to W^{0,\infty}_{r_0,n-2} \to W^{0,\infty}_{r_0,\log} \to C^0 \to C^0 \to \cdots, \quad \text{for } n = 2, 4, 6, \ldots, \tag{3.65d}$$

$$W^{0,\infty}_{r_0,2} \to W^{0,\infty}_{r_0,4} \to \cdots \to W^{0,\infty}_{r_0,n-1} \to C^0 \to C^0 \to \cdots, \quad \text{for } n = 3, 5, 7, \ldots. \tag{3.65e}$$

Let the normed space $B = L^\infty, L^p(p \ge 1), W^{0,\infty}_{r_0,2}(n \ge 3), W^{0,\infty}_{r_0,\log}(n = 2)$. If the condition

$$\|\delta\mu_a\|_{L^\infty} < \frac{1}{C_{10}\omega_n U(n)} \tag{3.66}$$

holds, then $E^\infty\Phi$ exists for each representation given in (3.65), and $F^m\Phi$ converges to $E^\infty\Phi$ for $\Phi \in B$.

Proof. From (3.58a), (3.58b), (2.29), and using $L^\infty \subset L^p$ for all $p \ge 1$, we get the sequence of function spaces (3.65a). From (2.28) and (2.29), we obtain (3.65b) and (3.65c). From (3.58c)-(3.58g), (3.65d) and (3.65e) are derived. The sufficient condition (3.66) results from (3.60c). □

Thus, by Theorems 3.8 and 3.9, we have answered the three questions related to the Born expansion and the Born approximation when $\delta\kappa = 0$.

Let us investigate conditions (3.63) and (3.66) in more detail. C_6, $C_7(2, 2)(n = 3, 5, 6, \ldots)$, $C_8(2, 2)(n = 4)$, and C_{10} can be estimated by

$$C_6 \le 1, \tag{3.67a}$$

$$C_7(2, 2) \le 2^{n-4}\left[\frac{3^{n-2}}{n-4} + 1\right], \quad n = 3, 5, 6, 7, \ldots, \tag{3.67b}$$

$$C_8(2, 2) \le 9 + \frac{1}{\log 2} \le 11, \quad n = 4, \tag{3.67c}$$

$$C_{10} \le 1.7d, \quad n = 2, \tag{3.67d}$$

$$C_{10} \le \frac{d^2}{2}, \quad n \ge 3. \tag{3.67e}$$

If we neglect the lower order term $R - H$, then the approximation of $U(n)$ is as follows:

$$U(n) \approx \sup_{r\in\Omega} |r - r_0|^{n-2}|H(r, r_0)| \le \frac{1}{(n-2)\omega_n L}, \quad n \ge 3, \tag{3.68}$$

$$U(n) \approx \sup_{r\in\Omega} |H(r, r_0)|/\log(|r - r_0|/2d) \le \frac{1}{\omega_n L}, \quad n = 2. \tag{3.69}$$

Using (3.67) and (3.68), the conditions (3.63) and (3.66) for the mth order Born approximation to converge to the Born expansion can be changed as follows :

$$\begin{aligned}
&\|\delta\mu_a\|_{L^\infty} \le \frac{L}{1.7d}, \quad n = 2 \text{ for (3.62b) and (3.65)},\\
&\|\delta\mu_a\|_{L^\infty} \le \frac{2(n-2)L}{d^2}, \quad n \ge 3 \text{ for (3.62b) and (3.65)},\\
&\|\delta\mu_a\|_{L^\infty} \le \frac{(n-2)(n-4)L}{2^{n-4}(3^{n-2}+n-4)}, \quad n = 3, 5, 6, \ldots, \text{ for (3.62c)},\\
&\|\delta\mu_a\|_{L^\infty} \le \frac{2L}{11}, \quad n = 4 \text{ for (3.62c)},\\
&\|\delta\mu_a\|_{L^\infty} \le \frac{L}{\log 2}, \quad n = 2 \text{ for (3.62d)}.
\end{aligned} \tag{3.70}$$

Note that all the condition in (3.70) depend on L, which is the lower bound of κ. Given the bound of C_1, a similar analysis can be obtained for the representation of the Born expansion in (3.62a).

4. The Fréchet derivatives

In this section, we derive the Fréchet derivatives of the coefficient-to-solution and the coefficient-to-measurement operators in Sections 4.1 and 4.2, respectively. In Section 4.3, we will argue some applications of the Fréchet derivative to DOT imaging. We consider the cases where the Born expansion has the infinite order representation with an index $M = 1$ such that

$$B \to B \to B \to \cdots, \tag{4.71}$$

where $B = W^{1,p}$ when both the diffusion and absorption coefficients are perturbed (Theorem 3.5) and $B = L^p, L^\infty, W^{0,\infty}_{r,2}$, or $W^{0,\infty}_{r,\log}$ when $\delta\kappa = 0$ (Theorem 3.8).

We first state the definition of the Fréchet derivative for operators defined on Banach spaces.

Let B_1 and B_2 be Banach spaces and $BL(B_1, B_2)$ be the Banach space of the bounded linear operators from B_1 to B_2 with a norm of

$$\|Q\|_{BL(B_1,B_2)} = \sup_{\mu\in B_1\setminus\{0\}} \frac{\|Q\mu\|_{B_2}}{\|\mu\|_{B_1}}, \quad Q \in BL(B_1, B_2). \tag{4.72}$$

Definition 4.1 (*The (First Order) Fréchet Derivative*)**.** Let S be an open set contained in B_1 and $P : S \subset B_1 \to B_2$ be an operator from S into B_2. Then, P is considered to be Fréchet differentiable for $\mu \in S$, if there is a continuous linear operator $Q : B_1 \to B_2$ such that

$$\lim_{\|\delta\mu\|_{B_1}\to 0} \frac{\|P(\mu+\delta\mu) - P(\mu) - Q(\delta\mu)\|_{B_2}}{\|\delta\mu\|_{B_1}} = 0. \tag{4.73}$$

The linear operator Q is called the first order Fréchet derivative of P and denoted by $P'(\mu)$.

Before moving to the mth order Fréchet derivative, we will introduce the second order Fréchet derivative to familiarize the reader with the idea of higher order derivatives.

Definition 4.2 (*The Second Order Fréchet Derivative*)**.** Let $P'(\mu) : B_1 \to B_2$ be the Fréchet derivative of $P : S \subset B_1 \to B_2$ at $\mu \in S$. Then $P' : S \subset B_1 \to BL(B_1, B_2)$. If P' is Fréchet differentiable at μ, we denote it by

$$P''(\mu) : B_1 \to BL(B_1, B_2). \tag{4.74}$$

And $P''(\mu)$ is called the second order Fréchet derivative or Hessian of P at $\mu \in S$. The operator P'' is defined as $P'' : S \to BL(B_1, BL(B_1, B_2))$.

Let us denote that $BL(B_1^m, B_2) = BL(B_1, BL(B^{m-1}, B_2))$, where $m = 2, 3, 4, \ldots$ and $BL(B_1^1, B_2) = BL(B_1, B_2)$. Then P'' is defined as an operator from $S \subset B_1$ to $BL(B_1^2, BL(B_1, B_2))$.

Definition 4.3 (*The mth Order Fréchet Derivative*)**.** Higher order Fréchet derivatives are defined recursively for $m = 3, \ldots$ by $P^{(m)}(\mu) : B_1 \to BL(B_1^{m-1}, B_2)$ such that

$$\lim_{\|\delta\mu\|_{B_1}\to 0} \frac{\left\|P^{(m-1)}(\mu+\delta\mu) - P^{(m-1)}(\mu) - P^{(m)}(\mu)\delta\mu\right\|_{BL(B_1^{m-1},B_2)}}{\|\delta\mu\|_{B_1}} = 0. \tag{4.75}$$

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We can also view $P^{(m)}(\mu)$ as a mapping from B_1^m (the Cartesian product of B_1 with itself m times) to B_2. Let us denote the image of $P^{(m)}(\mu)$ at m-tuples $(\delta\mu_1, \delta\mu_2, \ldots, \delta\mu_m) \in B_1^m$ by $P^{(m)}(\mu)[\delta\mu_1, \delta\mu_2, \ldots, \delta\mu_m]$. Let $P^{(m)}(\mu;\delta\mu) := P^{(m)}(\mu)[\delta\mu, \delta\mu, \ldots, \delta\mu]$ and $\frac{\partial^m P}{\partial\mu^m}(\delta\mu) = P^{(m)}(\mu;\delta\mu)$.

4.1. The Fréchet derivatives of the coefficient-to-solution operator

In Section 3, $\mathcal{R}^m = \mathcal{R}^m(\delta\mu)(\cdot)$ is treated as a bounded linear operator in $BL(B, B)$ mapping $\Phi \in B$ to $\mathcal{R}^m(\delta\mu)\Phi \in B$ with a given $\delta\mu$. However, in this section, we will interpret $\mathcal{R}^m = \mathcal{R}^m[\mu](\cdot)\Phi$ as an operator in $BL(G^m, B)$ such that

$$\mathcal{R}^m[\mu](\delta\mu_1, \delta\mu_2, \ldots, \delta\mu_m)\Phi = \mathcal{R}[\mu](\delta\mu_1)\mathcal{R}[\mu](\delta\mu_2)\cdots\mathcal{R}[\mu](\delta\mu_m)\Phi. \tag{4.76}$$

The notation $\mathcal{R}[\mu]$ is used instead of $\mathcal{R}$ to clarify the Robin function $R(r, r')$, the kernel of $\mathcal{R}[\mu]$, is defined with respect to the optical coefficient μ.

Then, by a similar analysis as in Theorems 3.5 and 3.8, we can show that the operator $\mathcal{R}^m\Phi$ is bounded for the operator norm from G^m into B such that

$$\left\| \mathcal{R}^m[\mu](\delta\mu_1, \ldots, \delta\mu_m)\Phi \right\|_{G^m\to B} \le C_{14} \|\delta\mu_1\|_G \cdots \|\delta\mu_m\|_G \|\Phi\|_B . \tag{4.77}$$

where $C_{14} = \max(C_4, C_5)$, C_5, and $C_{11}(B)$ depending on G and B defined in (1.14a), (1.14b), and (1.14c), respectively. Note that C_{14} remains fixed when μ is replaced by $\widetilde{\mu} = \mu + \delta\mu = (\kappa + \delta\kappa, \mu_a + \delta\mu_a)$, if $\widetilde{\mu}$ satisfies (1.2) with the same constants L and U. The second equation in (1.13) is interpreted as follows:

$$\mathcal{R}[\mu + \delta\mu] - \mathcal{R}[\mu] = \mathcal{R}^2[\mu]\delta\mu + \mathcal{R}^2[\mu]\mathcal{R}[\mu + \delta\mu]\delta\mu^2, \tag{4.78}$$

where the equation holds for all $q \in H^{-1}(\Omega)$ or q is a Dirac delta function. Using (4.77), we obtain

$$\mathcal{R}[\mu + \delta\mu] - \mathcal{R}[\mu] = \mathcal{R}^2[\mu]\delta\mu + o(\|\delta\mu\|_G). \tag{4.79}$$

Here $\psi = o(\|\delta\mu\|_G)$ for a bounded linear function $\psi \in BL(G^k, B)$ means that $\lim_{\|\delta\mu\|_G\to 0} \frac{\|\psi\|_{BL(G^k,B)}}{\|\delta\mu\|_G} = 0$.

Note that in the Born expansion, the mth order term is given by $\mathcal{R}^m[\mu](\delta\mu)\Phi$. The mth order Fréchet derivative corresponds to mth term of the Born expansion via Theorem 1.1. The proof of Theorem 1.1 will be given in this section:

Proof of Theorem 1.1. *We will prove that*

$$\mathcal{R}^m[\mu + \delta\mu] - \mathcal{R}^m[\mu] = m\mathcal{R}^{m+1}[\mu]\delta\mu + o(\|\delta\mu\|_G), \tag{4.80}$$

for a positive integer m. We already proved that (4.80) for $m = 1$ at (4.79). Suppose that (4.80) hold for all positive integers $i < m$, then

$$\begin{aligned}\mathcal{R}^m[\mu + \delta\mu] - \mathcal{R}^m[\mu] &= \sum_{i=0}^{m-1} \mathcal{R}^i[\mu + \delta\mu]\left[\mathcal{R}[\mu + \delta\mu] - \mathcal{R}[\mu]\right]\mathcal{R}^{m-1-i}[\mu] \\ &= \sum_{i=0}^{m-1} \mathcal{R}^i[\mu + \delta\mu]\mathcal{R}^{m+1-i}[\mu]\delta\mu + o(\|\delta\mu\|_G) \\ &= \sum_{i=0}^{m-1} \left[\mathcal{R}^i[\mu] + i\mathcal{R}^{i+1}\delta\mu + o(\|\delta\mu\|_G)\right]\mathcal{R}^{m+1-i}[\mu] + o(\|\delta\mu\|_G) \\ &= m\mathcal{R}^{m+1}[\mu]\delta\mu + o(\|\delta\mu\|_G).\end{aligned} \tag{4.81}$$

Therefore, we proved (4.80) by induction argument. Using (4.81), we obtain

$$\begin{aligned}\frac{\partial^{m-1}\Psi}{\partial\mu^{m-1}}(\mu + \delta\mu) - \frac{\partial^{m-1}\Psi}{\partial\mu^{m-1}}(\mu) &= (m-1)!\left[\mathcal{R}^{m-1}[\mu + \delta\mu]\widetilde{\Phi} - \mathcal{R}^{m-1}[\mu]\Phi\right] \\ &= (m-1)!\left[\mathcal{R}^m[\mu + \delta\mu] - \mathcal{R}^m[\mu]\right] q \\ &= (m-1)!mR^{m+1}[\mu]\delta\mu\, q + o(\|\delta\mu\|_G) \\ &= m!R^m[\mu]\delta\mu\Phi + o(\|\delta\mu\|_G).\end{aligned} \tag{4.82}$$

Using the definition of the higher order derivatives in (4.75), we obtained (1.15a). With a similar argument and noting that $\mathcal{R}_1$ is independent of $\delta\kappa$ and that $\mathcal{R}_2$ is independent of $\delta\mu_a$, we can prove (1.15b). □

If P is m-times continuously differentiable on S, and $P^{(m)}(\mu)$ is integrable between any two points in S, then the Taylor's theorem holds: For any $\mu, \mu + \delta\mu \in S$, we have

$$P(\mu + \delta\mu) = P(\mu) + \sum_{i=1}^{m-1} \frac{P^{(i)}(\mu)}{i!}\delta\mu^i + E_m(\mu + \delta\mu, \mu; P), \tag{4.83}$$

where

$$\|E_m(\mu+\delta\mu,\mu;P)\|_{B_2} \le \frac{\|\delta\mu\|_{B_1}^m}{m!} \sup_{\theta\in[0,1]} \left\|P^{(m)}(\mu+\theta\delta\mu)\right\|_{BL(B_1^{(m)},B_2)}. \tag{4.84}$$

Although the statement and proof are similar to the Taylor's theorem in Euclidean space, we must consider each term with respect to the operators between Banach spaces. For the proof of (4.83), see [43]. If another operator Q is m-times differentiable, $E_m(\mu+\delta\mu,\mu;Q) \le C\,\|\delta\mu\|_{B_1}^m$, and $P(\mu)=Q(\mu)$, then we can show that

$$P^{(i)}(\mu) = Q^{(i)}(\mu), \quad i=0,\dots,m-1. \tag{4.85}$$

Let $T^m := P(\mu)+\sum_{i=1}^m \frac{P^{(i)}(\mu)}{i!}\delta\mu^i$ be the mth order Taylor expansion. Then from Lemma 4.3 and (4.85), we conclude that the mth order Born approximation is the same as the mth order Taylor expansion, i.e. $T^m = F^m$. This fact can be used as another proof of Theorem 1.1 under the condition that Taylor order expansion is possible.

4.2. The Fréchet derivatives of the coefficient-to-measurement operator

In this subsection, we compute the Fréchet derivatives of the coefficient-to-measurement operator Γ.

Given the photon density function Φ, which is the solution of (1.1), different types of boundary data can be measured. Let f be any function from complex space $\mathbb{C}$ to complex space $\mathbb{C}$ and let $\Gamma = f(\Psi)$. The Fréchet derivatives of the coefficient-to-measurement operator Γ can be computed using the Fréchet derivatives of the coefficient-to-solution operator Ψ by using a change of variables as follows:

$$\Gamma' = f'(\Psi)\Psi' = f'(\Psi)\mathcal{R}\Phi,$$
$$\Gamma'' = f''(\Psi)(\Psi')^2 + f'(\Psi)\Psi'' = f''(\Psi)(\mathcal{R}\Phi)^2 + 2f'(\Psi)\mathcal{R}^2\Phi,$$

and

$$f(\Psi)^{(m)} = \sum_{i=1}^{m} f^{(i)}(\Psi)A_{m,i}(\mathcal{R}\Phi,\mathcal{R}^2\Phi,\dots,\mathcal{R}^{(m)}\Phi), \quad m\ge 3, \tag{4.86}$$

where $A_{m,i}$ is a polynomial of degree m and $A_{m,i}(x_1,\dots,x_m)$ is a linear combination of monomials $\Pi_{l=1}^m x_l^{j_l}$ with $\sum_{l=1}^m lj_l = m$, if f is m times differentiable.

The most widely used functions for f are

$$f(x) = \Re(x), \tag{4.87a}$$
$$f(x) = \Re(\log x), \tag{4.87b}$$

where $\Re(x)$ is the real part of complex number x. (4.87a) is called the Born measurement and (4.87b) is called the Rytov measurement.

In the case of the Born measurements, $\Gamma^{(m)} = m!\Re(\mathcal{R}^m\Phi)$, and in the case of Rytov measurement, the first and second order Fréchet derivatives are given by

$$\Gamma' = \Re\left(\frac{\mathcal{R}\Phi}{\Phi}\right), \tag{4.88a}$$

$$\Gamma'' = \Re\left(\frac{-(\mathcal{R}\Phi)^2}{\Phi^2} + \frac{2\mathcal{R}^2\Phi}{\Phi}\right). \tag{4.88b}$$

4.3. Applications

In [25], we proved the local convergence of a method which we call Two-level Multiplicative Space Decomposition Method for DOT image reconstruction. In the proof of the convergence, we assumed that the second order Fréchet derivative of the coefficient-to-measurement operator is bounded, when Rytov measurements are used. By using (4.77) and (4.88b), the second order Fréchet derivative is bounded by

$$\left\|\Gamma''\right\|_{G^2\to B} \le 3C_{14}^2, \tag{4.89}$$

when both the absorption and diffusion coefficients are perturbed.

In [7], inverse scattering series is used to invert Born expansion to consider higher order terms. (By Theorem 1.1 the Born expansion is the same as (1.7).) Then the idea of the inverse scattering series is as follows:

1. Find μ^+ by solving the first order Born approximation :

$$\Upsilon - \Gamma(\mu^0) = \mathcal{R}\Phi(\delta\mu^\dagger). \tag{4.90}$$

Let us assume that there exists a bounded operator $(\mathcal{R}\Phi)^\dagger$ from B to G such that $(\mathcal{R}\Phi)^\dagger(\mathcal{R}\Phi) = id_G$. We will call $(\mathcal{R}\Phi)^\dagger$ the left inverse of $\mathcal{R}\Phi$. Then we get the following expression for $\delta\mu^\dagger$

$$\delta\mu^\dagger = (\mathcal{R}\Phi)^\dagger \left[\Upsilon - \Gamma(\mu^0)\right]. \tag{4.91}$$

2. If we operate $(\mathcal{R}\Phi)^\dagger$ on both sides of (1.13), we obtain

$$\delta\mu = \delta\mu^\dagger - (\mathcal{R}\Phi)^\dagger\mathcal{R}^2(\delta\mu)^2\Phi - (\mathcal{R}\Phi)^\dagger\mathcal{R}^3(\delta\mu)^3\Phi - \cdots. \tag{4.92}$$

3. If we further approximate $\delta\mu$ in the right hand side of (4.92) as $\delta\mu^\dagger$, then we approximate $\delta\mu$ in the left hand side of (4.92) as $\delta\mu^i$. As a result, the implicit Eq. (4.92) is changed into the following explicit equation:

$$\delta\mu^i = \delta\mu^\dagger - (\mathcal{R}\Phi)^\dagger\mathcal{R}^2(\delta\mu^\dagger)^2\Phi - (\mathcal{R}\Phi)^\dagger\mathcal{R}^3(\delta\mu^\dagger)^3\Phi - \cdots, \tag{4.93}$$

where we will call $\delta\mu^i$ an inverse scattering series solution.

By (4.92), we get

$$\left\|\delta\mu - \delta\mu^\dagger\right\|_G \le \left\|(\mathcal{R}\Phi)^\dagger\right\|_{B\to G}\|\Phi\|_B \frac{(C_{14}\|\delta\mu\|_G)^2}{1 - C_{14}\|\delta\mu\|_G} \le C^\dagger\|\delta\mu\|_G^2, \tag{4.94}$$

where

$$C^\dagger = 2C_{14}^2\left\|(\mathcal{R}\Phi)^\dagger\right\|_{B\to G}\|\Phi\|_B,$$

and we assumed that $\|\delta\mu\|_G \le \frac{1}{2C_{14}}$. By subtracting (4.93) from (4.92) and using (4.92), we get

$$\delta\mu - \delta\mu^i = (\mathcal{R}\Phi)^+\left[\left(\mathcal{R}^2(\delta\mu^\dagger)^2\Phi - \mathcal{R}^2(\delta\mu)^2\Phi\right) + \left(\mathcal{R}^3(\delta\mu^\dagger)^3\Phi - \mathcal{R}^3(\delta\mu)^3\Phi\right)\right] \tag{4.95}$$

The multilinear operator $\mathcal{R}$ satisfies the following equation:

$$\begin{aligned}\mathcal{R}^q(\delta\mu^\dagger)^q\Phi - \mathcal{R}^q(\delta\mu)^q\Phi &\le \left[\mathcal{R}^q(\delta\mu^\dagger,\ldots,\delta\mu^\dagger,\delta\mu^\dagger)\Phi - \mathcal{R}^q(\delta\mu^\dagger,\ldots,\delta\mu^\dagger,\delta\mu)\Phi\right]\\ &+ \left[\mathcal{R}^q(\delta\mu^\dagger,\ldots,\delta\mu^\dagger,\delta\mu)\Phi - \mathcal{R}^q(\delta\mu^\dagger,\ldots,\delta\mu,\delta\mu)\Phi\right] + \cdots\\ &+ \left[\mathcal{R}^q(\delta\mu^\dagger,\ldots,\delta\mu,\delta\mu)\Phi - \mathcal{R}^q(\delta\mu,\ldots,\delta\mu,\delta\mu)\Phi\right].\end{aligned} \tag{4.96}$$

By (4.94), (4.96), and the multilinear property of $\mathcal{R}\Phi$, we obtain the following bound:

$$\begin{aligned}\left\|\mathcal{R}^q(\delta\mu^\dagger)^q\Phi - \mathcal{R}^q(\delta\mu)^q\Phi\right\|_B &\le \|\mathcal{R}\|_{G\to B}\|\Phi\|_B\left\|\delta\mu^\dagger - \delta\mu\right\|_G\cdot\left[\|\delta\mu\|_G^{q-1} + \|\delta\mu\|_G^{q-2}\left\|\delta\mu^\dagger\right\|_G + \cdots + \left\|\delta\mu^\dagger\right\|_G^{q-1}\right]\\ &\le \|\mathcal{R}\|_{G\to B}\|\Phi\|_B C^\dagger\|\delta\mu\|_G^{q+1}\left[1 + (1+C^\dagger) + \cdots + (1+C^\dagger)^{q-1}\right]\\ &\le \|\mathcal{R}\|_{G\to B}\|\Phi\|_B\|\delta\mu\|_G^{q+1}(1+C^\dagger)^q.\end{aligned} \tag{4.97}$$

Using (4.95)–(4.97), the error of the inverse scattering solution is given by

$$\begin{aligned}\left\|\delta\mu - \delta\mu^i\right\|_G &\le \left\|(\mathcal{R}\Phi)^+\right\|_{B\to G}\|\mathcal{R}\|_{G\to B}\|\Phi\|_B C^\dagger\|\delta\mu\|_G^3(1+C^\dagger)^2\cdot\left[1 + (1+C^\dagger)\|\delta\mu\|_G + (1+C^\dagger)^2\|\delta\mu\|_G^2 + \cdots\right]\\ &\le \left\|(\mathcal{R}\Phi)^+\right\|_{B\to G}\|\mathcal{R}\|_{G\to B}\|\Phi\|_B\|\delta\mu\|_G^3(1+C^\dagger)^2\frac{1}{1-(1+C^\dagger)\|\delta\mu\|_G}\\ &\le \widetilde{C}\|\delta\mu\|_G^3,\end{aligned} \tag{4.98}$$

where $\|\delta\mu\|_G \le \frac{1}{2(1+C^\dagger)}$ and $\widetilde{C} := 2(1+C^\dagger)^2\left\|(\mathcal{R}\Phi)^+\right\|_{B\to G}\|\mathcal{R}\|_{G\to B}\|\Phi\|_B$. The error of the inverse scattering series solution $\delta\mu^i$ in (4.98) is of the order $O(\|\delta\mu\|_G^3)$, which is a higher order than the order of the error of the linearized solution $O(\|\delta\mu\|_G^2)$.

5. Conclusion

In this paper, we derived the Born expansion and Fréchet derivatives for the Diffuse Optical Tomography for arbitrary domains with Robin type boundary conditions. To analyze the Born expansion, we introduced sequences of appropriate normed spaces such as Lebesgue spaces, Sobolev spaces, and weighted Sobolev spaces. We derived sufficient conditions on the perturbation in the diffusion and absorption coefficients for the convergence of the Born expansion in n dimensions, $(n \ge 2)$. We computed bounds for the error in the mth order Born approximation. Next, we showed that the mth order Fréchet derivatives of the coefficient-to-solution operator is equal to $m!$ times the mth corresponding term in the Born expansion. This analysis is applied to the inverse scattering series [7] and the convergence of domain decomposition method in DOT [25].

Although we only consider the boundary value problem (2.1) with Robin boundary conditions, the analysis introduced in this paper can be easily extended to the general second order elliptic partial differential equations with other boundary conditions.

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Appendix A. Proof of Lemma 2.2

Using $W^{0,\infty}_{r,\alpha} \subset W^{0,\infty}_{r,\alpha-\epsilon}$ for all $0 \le \epsilon < \alpha$, $L(r,\cdot) \in W^{0,\infty}_{r,2-\epsilon}$ and inserting $q = p$ into (2.27), we get (2.32a) with a constant $C_1(\min\left(\frac{n}{p}-\epsilon, 2-\epsilon\right), p, p)$. Using $\frac{\partial L(r',\cdot)}{\partial r_i} \in W^{0,\infty}_{r',1}$ and inserting $q = p$, we get (2.33a) and (2.32c)with a constant $C_1(\min\left(\frac{n}{p}, 1\right), p, p)$.

We can start to prove (2.32d) and (2.33b) by defining

$$v_{i,\delta}(r) := \int_{\Omega\setminus\bar{B}(r,\delta)} \frac{\partial H(r,r')}{\partial r_i}\psi(r')\mathrm{d}r'. \tag{A.99}$$

Taking the derivative of $v_{i,\delta}$, we get

$$\begin{aligned}\frac{\partial v_{i,\delta}}{\partial r_j}(r) &= \int_{\Omega\setminus\bar{B}(r,\delta)} \frac{\partial^2 H(r,r')}{\partial r_i \partial r_j}\psi(r')\mathrm{d}r' - \int_{\partial B(r,\delta)} \frac{\partial H(r,r')}{\partial r_i}\psi(r')\nu_j^\delta \mathrm{d}S(r') \\ &= \psi(r)\int_{\partial B(r,\delta)} \frac{\partial H(r,r')}{\partial r_i}\nu_j^\delta \mathrm{d}S(r') + \int_{\Omega\setminus\bar{B}(r,\delta)} \frac{\partial^2 H(r,r')}{\partial r_i\partial r_j}\psi(r')\mathrm{d}r' \\ &\quad - \int_{\partial B(r,\delta)}\left[\frac{\partial H(r,r')}{\partial r_i}\psi(r') + \frac{\partial H(r',r)}{\partial r_i}\psi(r)\right]\nu_j^\delta \mathrm{d}S(r'),\end{aligned} \tag{A.100}$$

where ν_j^Ω and ν_j^δ are the jth component of the outer normal vector with respect to $\partial\Omega$ and $\partial B(r,\delta)$, respectively. Let us assume $\psi \in C^{0,\lambda}$. Using $\frac{\partial(H(r',\cdot)+H(\cdot,r'))}{\partial r_i} r_j \in W^{0,\infty}_{r',1+\lambda}$ the integral in the last line of (A.100) is bounded by

$$\begin{aligned}&\left|\int_{\partial B(r,\delta)}\left[\frac{\partial H(r,r')}{\partial r_i}\psi(r') + \frac{\partial H(r',r)}{\partial r_i}\psi(r)\right]\nu_j^\delta \mathrm{d}S(r')\right| \le \int_{\partial B(r,\delta)}\left|\frac{\partial(H(r,r')+H(r',r))}{\partial r_i}\psi(r')\right|\mathrm{d}S(r') \\ &\quad + \int_{\partial B(r,\delta)}\left|\frac{\partial H(r',r)}{\partial r_i}\right|\left|\psi(r')-\psi(r)\right|\mathrm{d}S(r') \le \frac{\delta^\lambda}{\lambda}\omega_n\|\psi\|_{C^{0,\lambda}}\left[\frac{\|\kappa\|_{C^{0,\lambda}}}{nL^2} + \frac{1}{nL}\right].\end{aligned} \tag{A.101}$$

Thus, by (A.101), the integral in the last line of (A.100) goes to zero as δ goes to zero for $\psi \in C^{0,\lambda}$. And the first integral in the second last line (A.100) is $-\psi(r)\frac{1}{n\kappa(r)}$. Letting δ go to zero, we get

$$\begin{aligned}\frac{\partial^2 v}{\partial r_i\partial r_j}(r) &= \int_\Omega \frac{\partial^2(L-H)(r,r')}{\partial r_i\partial r_j}\psi(r')\mathrm{d}r' + \lim_{\delta\to 0}\frac{\partial v_{i,\delta}}{\partial r_j}(r) \\ &= \int_\Omega \frac{\partial^2(L-H)(r,r')}{\partial r_i\partial r_j}\psi(r')\mathrm{d}r' + \int_\Omega \frac{\partial^2 H(r,r')}{\partial r_i\partial r_j}\psi(r')\mathrm{d}r' - \frac{\psi(r)}{n\kappa(r)}.\end{aligned} \tag{A.102}$$

The second integral of the right hand side of (A.102) is bounded in the sense of (2.30). Thus we have proved (2.33b). Let us prove (2.32d) using (2.27), (2.30) and (A.102).

$$\left\|\frac{\partial^2 v}{\partial r_i\partial r_j}\right\|_{L^p} \le C_1(\lambda,p,p)\|\psi\|_{L^p}\sup_{r'\in\Omega}\left\|\frac{\partial^2(L-H)(r',\cdot)}{\partial r_i\partial r_j}\right\| + \frac{C_3}{L}\|\psi\|_{L^p} + \frac{1}{nL}\|\psi\|_{L^p}. \tag{A.103}$$

Thus, we proved (2.32d) for $\psi \in C^{0,\lambda}$. An extension of (2.32d) when $\phi \in L^p$ can be found in [16,35]. (2.33c) follows from (2.33a) and (2.33b). To prove (2.34), using Stokes theorem in $\Omega \setminus B(r,\delta)$, we get

$$\begin{aligned}&\int_{\Omega\setminus B(r,\delta)}\left[v(r')\mathcal{M}_{r'}L(r,r') - L(r,r')\mathcal{M}_{r'}v(r')\right]\mathrm{d}r' = \int_{\partial\Omega}\left[v(r')\mathcal{N}_{r'}L(r,r') - L(r,r')\mathcal{N}_{r'}v(r')\right]\mathrm{d}S(r') \\ &\quad - \int_{\partial B(r,\delta)}\left[v(r')\kappa(r')\frac{\partial L(r,r')}{\partial\nu_{r'}} - L(r,r')\kappa(r')\frac{\partial v(r')}{\partial\nu}\right]\mathrm{d}S(r').\end{aligned} \tag{A.104}$$

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Since $v \in W^{2,p}(\Omega)$, $v \in W^{2-\frac{1}{p},p}(\partial\Omega)$ by trace formula, each term of the second integral of the right hand side of (A.104) has the following asymptotic behavior:

$$\left|\int_{\partial B(r,\delta)} L(r,r')\kappa(r')\frac{\partial v}{\partial \nu}(r')\mathrm{d}S(r')\right| \le U\,\|L(r,\cdot)\|_{W^{0,\infty}_{r,2}}\,\|v\|_{W^{2,p}}, \tag{A.105a}$$

$$\left|\int_{\partial B(r,\delta)} v(r')\kappa(r')\frac{\partial(L-H)(r,r')}{\partial \nu}(r')\mathrm{d}S(r')\right| \le U\,\|v\|_{W^{2,p}}\left\|\frac{\partial(L-H)(r,\cdot)}{\partial r'_i}\right\|_{W^{0,\infty}_{r,1+\lambda}}\delta^{\lambda}, \tag{A.105b}$$

$$\int_{\partial B(r,\delta)} v(r')\kappa(r')\frac{\partial H(r,r')}{\partial \nu}(r')\mathrm{d}S(r') = \int_{\partial B(r,1)} v\left(\delta\frac{r'-r}{|r'-r|}\right)\mathrm{d}S\left(\frac{r'-r}{|r'-r|}\right). \tag{A.105c}$$

(A.105a) and (A.105b) go to 0 as δ goes to 0 and (A.105c) goes to $v(r)$ as δ goes to 0 by the mean value theorem. Thus, letting $\delta \to 0$ and combining (A.104) and (A.105), we get (2.34), where the first term in (A.104) is interpreted in the same manner as in (2.30). □

Appendix B. Proof of Lemma 3.6

(3.58a) and (3.58b) are obtained easily using spherical coordinates with respect to r^1. Let us divide Ω into three regions, depending on the two points r^1 and r^2:

$$\Omega_{r^1} = \left\{r' \in \Omega \,\middle|\, |r'-r^1| \le \frac{|r^1-r^2|}{2}\right\},$$

$$\Omega_{r^2} = \left\{r' \in \Omega \,\middle|\, |r'-r^2| \le \frac{|r^1-r^2|}{2}\right\},$$

$$\Omega_{c} = \left\{r' \in \Omega \,\middle|\, |r'-r^1| > \frac{|r^1-r^2|}{2}, |r'-r^2| > \frac{|r^1-r^2|}{2}\right\}.$$

Consider the Eq. (3.58c), which is decomposed as

$$\begin{aligned}\int_{\Omega} \log(2d/|r^1-r'|)\log(2d/|r^2-r'|)\mathrm{d}r' &= \int_{\Omega_{r^1}} \log(2d/|r^1-r'|)\log(2d/|r^2-r'|)\mathrm{d}r' \\ &+ \int_{\Omega_{r^2}} \log(2d/|r^1-r'|)\log(2d/|r^2-r'|)\mathrm{d}r' + \int_{\Omega_c} \log(2d/|r^1-r'|)\log(2d/|r^2-r'|)\mathrm{d}r'.\end{aligned} \tag{B.106}$$

Next, consider the first term in the right hand side of (B.106). If $r' \in \Omega_{r^1}$, then $|r'-r^2| \ge \frac{|r^1-r^2|}{2}$. Then, by a change of variables with respect to the spherical coordinates centered at r^1, we get

$$\begin{aligned}\int_{\Omega_{r^1}} \log(2d/|r^1-r'|)\log(2d/|r'-r^2|)\mathrm{d}r' &\le \omega_2 \log(4d/|r^1-r^2|)\int_0^{\frac{|r^1-r^2|}{2}} \rho\log(2d/\rho)\mathrm{d}\rho \\ &\le \frac{\omega_2}{16}\log(4d/|r^1-r^2|)|r^1-r^2|^2[2\log(4d/|r^1-r^2|)+1].\end{aligned} \tag{B.107}$$

Likewise,

$$\int_{\Omega_{r^2}} \log(2d/|r^1-r'|)\log(2d/|r'-r^2|)\mathrm{d}r' \le \frac{\omega_2}{16}\log(4d/|r^1-r^2|)|r^1-r^2|^2[2\log(4d/|r^1-r^2|)+1]. \tag{B.108}$$

If $r' \in \Omega_c$, then $|r^1-r'| \ge \frac{|r'-r^2|}{3}$. Then, by a change of variables with respect to spherical coordinates centered at r^2, we get

$$\begin{aligned}\int_{\Omega_c} \log(2d/|r^1-r'|)\log(2d/|r'-r^2|)\mathrm{d}r' &\le \int_{\Omega_c} \log(6d/|r'-r^2|)\log(2d/|r'-r^2|)\mathrm{d}r' \\ &\le \omega_2\int_0^d (\log 3\log(2d/\rho) + (\log(2d/\rho))^2)\rho\mathrm{d}\rho \\ &\le \omega_2 d^2\left[\frac{1}{2}(\log 2)^2 + \frac{1}{4}(\log 3 - 1)(2\log 2 + 1)\right].\end{aligned} \tag{B.109}$$

Inserting (B.107), (B.108), and (B.109) into (B.106), we get (3.58c).

Returning to (3.58b), (3.58d), and (3.58e), we get

$$\int_{\Omega} |r^1 - r'|^{\alpha_1 - n} |r' - r^2|^{\alpha_2 - n} \mathrm{d}r' = \int_{\Omega_{r1}} |r^1 - r'|^{\alpha_1 - n} |r' - r^2|^{\alpha_2 - n} \mathrm{d}r' + \int_{\Omega_{r2}} |r^1 - r'|^{\alpha_1 - n} |r' - r^2|^{\alpha_2 - n} \mathrm{d}r' + \int_{\Omega_c} |r^1 - r'|^{\alpha_1 - n} |r' - r^2|^{\alpha_2 - n} \mathrm{d}r', \quad \text{(B.110)}$$

where each term in the right hand side of (B.110) is bounded by

$$\begin{aligned}\int_{\Omega_{r1}} |r^1 - r'|^{\alpha_1 - n} |r' - r^2|^{\alpha_2 - n} \mathrm{d}r' &\le 2^{n-\alpha_2} |r^1 - r^2|^{\alpha_2 - n} \int_{\Omega_{r1}} |r^1 - r'|^{\alpha_1 - n} \mathrm{d}r' \\ &\le 2^{n-\alpha_2} |r^1 - r^2|^{\alpha_2 - n} \int_0^{|r^1 - r^2|/2} \rho^{\alpha_1 - n} \rho^{n-1} \omega_n \mathrm{d}\rho \\ &= \frac{\omega_n}{\alpha_1} 2^{n-\alpha_1-\alpha_2} |r^1 - r^2|^{\alpha_1 + \alpha_2 - n}. \end{aligned} \quad \text{(B.111)}$$

Likewise

$$\int_{\Omega_{r2}} |r^1 - r'|^{\alpha_1 - n} |r' - r^2|^{\alpha_2 - n} \mathrm{d}r' \le \frac{\omega_n}{\alpha_2} 2^{n-\alpha_1-\alpha_2} |r^1 - r^2|^{\alpha_1 + \alpha_2 - n}. \quad \text{(B.112)}$$

Suppose that $\alpha_1 + \alpha_2 < n$, then

$$\begin{aligned}\int_{\Omega_c} |r^1 - r'|^{\alpha_1 - n} |r' - r^2|^{\alpha_2 - n} \mathrm{d}r' &\le 3^{n-\alpha_1} \int_{\Omega_c} |r' - r^2|^{\alpha_1 + \alpha_2 - 2n} \mathrm{d}r' \\ &\le 3^{n-\alpha_1} \int_{|r^1 - r^2|/2}^{\infty} \rho^{\alpha_1 + \alpha_2 - 2n} \rho^{n-1} \omega_n \mathrm{d}\rho \\ &\le 3^{n-\alpha_1} 2^{n-\alpha_1-\alpha_2} |r^1 - r^2|^{\alpha_1 + \alpha_2 - n} \frac{\omega_n}{n - \alpha_1 + \alpha_2}. \end{aligned} \quad \text{(B.113)}$$

By inserting (B.111), (B.112), and (B.113) into (B.110) and considering the symmetry of r^1 and r^2 for (B.113), we get (3.58d). (3.58e) and (3.58f) are derived by modifying the integral area for the third integral in (B.113) into $\{r' \,\big|\, |r^1 - r^2| \le |r'| \le d\}$ and $\{r' \,\big|\, 0 \le |r'| \le d\}$, respectively, instead of Ω. Finally, (3.58g) is computed in a similar way as follows:

$$\begin{aligned}&\left| \int_{\Omega} |r^1 - r'|^{\alpha_1 - n} \log(2d/|r' - r^2|) \mathrm{d}r' \right| \le \int_{\Omega_{r1}} |r^1 - r'|^{\alpha_1 - n} |\log(2d/|r' - r^2|)| \mathrm{d}r' \\ &\quad + \int_{\Omega_{r2}} |r^1 - r'|^{\alpha_1 - n} |\log(2d/|r' - r^2|)| \mathrm{d}r' + \int_{\Omega_c} |r^1 - r'|^{\alpha_1 - n} |\log(2d/|r' - r^2|)| \mathrm{d}r' \\ &\le \omega_n \log(4d/|r^1 - r^2|) \frac{|r^1 - r^2|^{\alpha_1}}{\alpha_1 2^{\alpha_1}} + \omega_n \frac{|r^1 - r^2|^{\alpha_1}}{2^{\alpha_1} n} \left(\log(4d/|r^1 - r^2|) + \frac{1}{n} \right) \\ &\quad + \omega_n \frac{d^{\alpha_1}}{\alpha_1} \left(\log(6) + \frac{1}{\alpha_1} \right) \le \omega_n d^{\alpha_1} C_7(\alpha_1). \end{aligned}$$

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