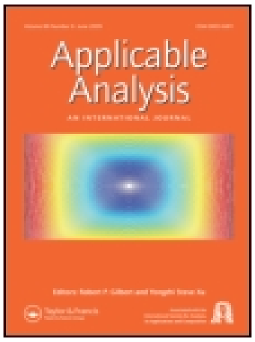

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A posteriori error analysis in radiative transfer

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The radiative transfer equation (RTE) arises in a wide variety of applications. In the literature, there has been much study of the RTE. The main purpose of the paper is to present a unified framework to develop a posteriori estimates for numerical solution errors and modeling errors, in an energy norm natural to the RTE problem. The derivation of the error estimates is through duality arguments. A posteriori error estimates in an L^2 norm are also presented, extending existing results available in the literature. The error estimates are completely computable in the sense that no unspecified constants are involved. A posteriori error estimates for numerical solutions are the basis for developing efficient adaptive solution algorithms, whereas a posteriori estimates for modeling errors are useful to analyze the effects of uncertainties in problem data on the solution.

Keywords: radiative transfer equation; weak formulation; variational principle; dual formulation; a posteriori error estimation; parity equation

AMS Subject Classifications: 65N15; 49S05

1. Introduction

The radiative transfer equation (RTE) arises in a wide variety of applications, such as astrophysics,[1] atmosphere and ocean,[2,3] heat transfer,[4] neutron transport,[5,6] optical molecular imaging,[7] and so on. Substantial research effort on the RTE began in the middle of last century. Today, research on the RTE remains to be a very active and important area, see e.g. the collections.[8,9] Recently, there is much interest in analysis and numerical simulation of the RTE and its related inverse problems, motivated by applications in biomedical optics.[10–16]

The model boundary value RTE problem considered in this paper is given by

$$\boldsymbol{\omega}\cdot\nabla u + \mu_t u - Su = f \quad \text{in } X \times \Omega, \tag{1.1}$$

$$u = u_{\text{in}} \quad \text{on } \Gamma_-. \tag{1.2}$$

Throughout the paper, we denote by X a C^1 domain in $\mathbb{R}^3$, and by Ω the unit sphere in $\mathbb{R}^3$. A generic point in X is denoted by $\boldsymbol{x}$, whereas a generic point in Ω is denoted by $\boldsymbol{\omega}$. The

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unknown function $u(\boldsymbol{x}, \boldsymbol{\omega})$ is the angular flux at the point $\boldsymbol{x}$ in the direction $\boldsymbol{\omega}$. The RTE (1.1) contains two medium parameters, the total cross section $\mu_t(\boldsymbol{x})$ and the differential scattering cross section $\mu_s(\boldsymbol{x}, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})$, which is the kernel function of the integral operator S:

$$Su(\boldsymbol{x}, \boldsymbol{\omega}) = \int_\Omega \mu_s(\boldsymbol{x}, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\, u(\boldsymbol{x}, \hat{\boldsymbol{\omega}})\, d\hat{\boldsymbol{\omega}}. \tag{1.3}$$

The function $f(\boldsymbol{x}, \boldsymbol{\omega})$ represents a source density. We use $\Gamma = \partial X \times \Omega$ for the boundary of $X \times \Omega$, and Γ_- and Γ_+ for the incoming and outgoing parts of the boundary:

$$\Gamma_- := \{(\boldsymbol{x}, \boldsymbol{\omega}) \in \Gamma \mid \boldsymbol{\omega}\cdot\boldsymbol{\nu}(\boldsymbol{x}) < 0\},$$
$$\Gamma_+ := \{(\boldsymbol{x}, \boldsymbol{\omega}) \in \Gamma \mid \boldsymbol{\omega}\cdot\boldsymbol{\nu}(\boldsymbol{x}) > 0\},$$

where $\boldsymbol{\nu}(\boldsymbol{x})$ is the unit outward normal vector at $\boldsymbol{x} \in \partial X$. The relation (1.2) is an inflow boundary condition with a given inflow function u_{in}.

The RTE has been studied extensively, theoretically, and numerically. An early systematic mathematical study of the RTE problem is [17], where parity equation formulations were also introduced. In [5], solution existence for the boundary value problem (1.1)–(1.2) is shown by transforming it into an equivalent integral equation. In [18], a detailed treatment of the RTE through the semi-group theory is given. Variational formulations of the RTE are studied in detail in [19]. In [20], mixed variational formulations with different smoothness requirements on the even-parity solution component and odd-parity solution component are introduced and analyzed. The Ref. [21], written from an engineering perspective, contains a wealth of materials on optimal principles, complementary variational formulations, and numerical simulations of the RTE problems. One purpose of the present paper is to revisit some variational principles, dual formulations, and parity equations for the RTE through a concise approach, and to provide a solid mathematical foundation for all the relevant results. Precise function space settings will be introduced in the studies. The dual formulations will be derived based on the general framework presented in [22]. Parity formulations will be deduced directly from the weak formulation of the RTE problem. This approach eliminates the need to first figure out appropriate form of boundary conditions for the second-order form of the RTE. We will derive a posteriori error estimates for the effects of numerical discretizations and of uncertainties in the problem data. The error estimates will be given in a natural energy norm of the function space, where the solution is sought, as well as in the L^2 norm. For the former type of error estimates, the duality theory in convex analysis will be applied. The latter type of error estimates extend some existing results. A posteriori error estimates for numerical solutions are the basis for developing efficient adaptive solution algorithms, whereas a posteriori estimates for modeling errors are useful to analyze the effects of uncertainties in problem data on the solution.[23]

In the study of the boundary value problem of the RTE, we need some function spaces. Let

$$Q := L^2(X \times \Omega) \tag{1.4}$$

be the Hilbert space of measurable functions on $X \times \Omega$ with the inner product $(u, v)_Q := \int_{X\times\Omega} u\, v$ and norm $\|v\|_Q := (v, v)_Q^{1/2}$. Here and below, to simplify the notation for an integral, we usually do not explicitly display the infinitesimal volume or surface element which can be easily identified by the domain where the integration is taken. Denote by $L^2(\Gamma)$ the Hilbert space of functions v on Γ with the inner product $(u, v)_\Gamma := \int_\Gamma |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\, u\, v$

and norm $\|v\|_\Gamma := (v, v)_\Gamma^{1/2}$. Similarly, we define the spaces $L^2(\Gamma_\pm)$ with the inner products $(u, v)_{\Gamma_\pm} := \int_{\Gamma_\pm} |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\, u\, v$ and norms $\|v\|_{\Gamma_\pm} := (v, v)_{\Gamma_\pm}^{1/2}$. We will need the Hilbert space

$$V := \left\{ v \in L^2(X \times \Omega) \mid \boldsymbol{\omega}\cdot\nabla v \in L^2(X \times \Omega),\ v|_\Gamma \in L^2(\Gamma) \right\}. \tag{1.5}$$

This space will be endowed with an inner product natural to the boundary value problem (1.1)–(1.2) and the corresponding norm may be viewed as an energy norm; cf. Subsection 2.1.

We make the following assumptions on the data

$$\mu_t \in L^\infty(X) \quad \text{and} \quad \mu_t \ge \mu_0 > 0 \text{ a.e. in } X, \tag{1.6}$$

$$\mu_s \in L^\infty(X \times (-1, 1)) \quad \text{and} \quad \mu_s \ge 0 \text{ a.e. in } X \times (-1, 1), \tag{1.7}$$

$$\kappa := \operatorname*{ess\,sup}_{\boldsymbol{x}\in X} \frac{1}{\mu_t(\boldsymbol{x})} \int_\Omega \mu_s(\boldsymbol{x}, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\, d\hat{\boldsymbol{\omega}} < 1, \tag{1.8}$$

$$f \in L^2(X \times \Omega), \quad u_{\text{in}} \in L^2(\Gamma_-), \tag{1.9}$$

where μ_0 is a constant. For the assumption (1.8), note that

$$\int_\Omega \mu_s(\boldsymbol{x}, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\, d\hat{\boldsymbol{\omega}} = 2\pi \int_{-1}^{1} \mu_s(\boldsymbol{x}, t)\, dt$$

is independent of $\boldsymbol{\omega}$. It is well known [19] that the boundary value problem (1.1)–(1.2) has a unique solution in the space V.

The rest of the paper is organized as follows. In Section 2, we present a weak formulation and a variational principle of the boundary value problem (1.1)–(1.2), and show that the dual formulation of the variational formulation is itself. In Section 3, we provide two kinds of a posteriori error bounds. In the first kind, the error is measured in the energy norm of the space V, and the error bound is derived through an application of the duality theory in convex analysis. In the second kind, the error is measured in L^2 norms; the errors bounds are derived directly and they extend some existing a posteriori error estimates found in the literature. In Section 4, we consider the even-parity and odd-parity problems, which can be constructed from the weak formulation of the boundary value problem (1.1)–(1.2) in a straightforward manner. In Section 5, we show that the dual of the even-parity problem is the odd-parity problem, and the dual of the odd-parity problem is the even-parity problem. In Section 6, we apply the duality theory in convex analysis to derive a posteriori error estimates for numerical solution errors and modeling errors in even-parity and odd-parity problems. The paper ends with some concluding remarks in Section 7.

2. A variational principle and its dual

In this section, we consider a weak formulation and the corresponding variational principle of the boundary value problem (1.1)–(1.2). Then, we show that the dual formulation of the variational formulation is itself.

2.1. *A variational principle*

The RTE (1.1) is a first-order equation and thus itself is not the Euler equation of a variational principle. To introduce a variational formulation for the problem (1.1)–(1.2), we first formally convert (1.1) to a second-order equation. We define an operator $\Sigma : Q \to Q$ by the formula

$$\Sigma v := \mu_t v - S v, \quad v \in Q. \tag{2.1}$$

LEMMA 2.1 *Assume (1.6)–(1.8). Then for any $r \in \mathbb{R}$, the power $\Sigma^r : Q \to Q$ is well defined, and is bounded, self-adjoint, and Q-elliptic. Moreover,*

$$\|\Sigma^{-1}\| \le \frac{1}{(1-\kappa)\,\mu_0}, \quad \|\Sigma^{-1/2}\| \le \frac{1}{[(1-\kappa)\,\mu_0]^{1/2}}. \tag{2.2}$$

Proof First, we note that obviously, $\Sigma \in \mathcal{L}(Q)$ and is self-adjoint. Let us prove the Q-ellipticity of Σ. Consider the quantity $(\Sigma v, v)_Q = (\mu_t v, v)_Q - (Su, v)_Q$. Let us bound the term

$$(Sv, v)_Q = \int_X dx \int_{\Omega\times\Omega} \mu_s(\boldsymbol{x}, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\, v(\boldsymbol{x}, \hat{\boldsymbol{\omega}})\, v(\boldsymbol{x}, \boldsymbol{\omega})\, d\hat{\boldsymbol{\omega}}\, d\boldsymbol{\omega}.$$

Use the Cauchy–Schwarz inequality repeatedly,

$$\left|\int_{\Omega\times\Omega} \mu_s(\boldsymbol{x}, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\, v(\boldsymbol{x}, \hat{\boldsymbol{\omega}})\, v(\boldsymbol{x}, \boldsymbol{\omega})\, d\hat{\boldsymbol{\omega}}\, d\boldsymbol{\omega}\right| \le \left(\int_\Omega \mu_s(\boldsymbol{x}, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\, d\hat{\boldsymbol{\omega}}\right)\left(\int_\Omega v(\boldsymbol{x}, \boldsymbol{\omega})^2 d\boldsymbol{\omega}\right).$$

Hence, $(Sv, v)_Q \le \kappa(\mu_t v, v)_Q$, and

$$(\Sigma v, v)_Q \ge (1-\kappa)\,(\mu_t v, v)_Q \ge (1-\kappa)\,\mu_0 (v, v)_Q. \tag{2.3}$$

Thus, Σ is Q-elliptic.

Since $\Sigma : Q \to Q$ is bounded, self-adjoint, and Q-elliptic, for any $r \in \mathbb{R}$, $\Sigma^r : Q \to Q$ is well-defined, and is bounded, self-adjoint, and Q-elliptic.

The bounds (2.2) follow from (2.3). □

Thanks to Lemma 2.1, we can introduce the following inner product and norm in the space V:

$$(u, v)_V := \left(\Sigma^{-1}(\boldsymbol{\omega}\cdot\nabla u), \boldsymbol{\omega}\cdot\nabla v\right)_Q + (\Sigma u, v)_Q + (u, v)_\Gamma, \tag{2.4}$$

$$\|v\|_V := \left[\left\|\Sigma^{-1/2}(\boldsymbol{\omega}\cdot\nabla v)\right\|_Q^2 + \left\|\Sigma^{1/2}(v)\right\|_Q^2 + \|v\|_\Gamma^2\right]^{1/2}. \tag{2.5}$$

The norm $\|\cdot\|_V$ is equivalent to the canonical norm $\|\cdot\|_V$ over V. As we will see later, the inner product (2.4) is natural in the study of the RTE problem (1.1)–(1.2) and the norm (2.5) may be viewed as an energy norm.

From Equation (1.1), we have

$$u = \Sigma^{-1}(f - \boldsymbol{\omega}\cdot\nabla u). \tag{2.6}$$

Using this expression to rewrite the term $\boldsymbol{\omega}\cdot\nabla u$ in (1.1), we can formally write the RTE as a second-order equation

$$\boldsymbol{\omega}\cdot\nabla\Sigma^{-1}(f - \boldsymbol{\omega}\cdot\nabla u) + \Sigma u = f \quad \text{in } X\times\Omega. \tag{2.7}$$

To determine appropriate forms of boundary conditions for this second-order equation, we multiply Equation (2.7) by an arbitrary smooth function v, integrate over $X \times \Omega$, and perform an integration by parts,

$$\int_\Gamma \boldsymbol{\omega}\cdot\boldsymbol{\nu}\, \Sigma^{-1}(f - \boldsymbol{\omega}\cdot\nabla u)\, v + \int_{X\times\Omega} \left[-\Sigma^{-1}(f - \boldsymbol{\omega}\cdot\nabla u)\, \boldsymbol{\omega}\cdot\nabla v + \Sigma(u)\, v \right] = \int_{X\times\Omega} f\, v.$$

The boundary integral term is split into sub-integrals over Γ_+ and Γ_-; over Γ_+, we use the relation (2.6), whereas over Γ_-, we use the relation (2.6) and the boundary condition (1.2):

$$\int_\Gamma \boldsymbol{\omega}\cdot\boldsymbol{\nu}\, \Sigma^{-1}(f - \boldsymbol{\omega}\cdot\nabla u)\, v = \int_{\Gamma_+} |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\, u\, v + \int_{\Gamma_-} |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\, (u - 2\, u_{\text{in}})\, v.$$

Summarizing, we have derived the following weak formulation for the boundary value problem (1.1)–(1.2):

$$\begin{aligned} u \in V, \quad & \int_{X\times\Omega} \left[\Sigma^{-1}(\boldsymbol{\omega}\cdot\nabla u)\, \boldsymbol{\omega}\cdot\nabla v + \Sigma(u)\, v \right] + \int_\Gamma |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\, u\, v \\ & = \int_{X\times\Omega} \left[f\, v + \Sigma^{-1}(f)\, \boldsymbol{\omega}\cdot\nabla v \right] + 2 \int_{\Gamma_-} |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\, u_{\text{in}} v \quad \forall\, v \in V. \end{aligned} \tag{2.8}$$

Formally, the classical formulation of the problem (2.8) is

$$-\boldsymbol{\omega}\cdot\nabla\Sigma^{-1}(\boldsymbol{\omega}\cdot\nabla u) + \Sigma u = f - \boldsymbol{\omega}\cdot\nabla\Sigma^{-1}(f) \quad \text{in } X \times \Omega, \tag{2.9}$$

$$u + \Sigma^{-1}(\boldsymbol{\omega}\cdot\nabla u) = \Sigma^{-1}(f) \quad \text{on } \Gamma_+, \tag{2.10}$$

$$u - \Sigma^{-1}(\boldsymbol{\omega}\cdot\nabla u) = 2\, u_{\text{in}} - \Sigma^{-1}(f) \quad \text{on } \Gamma_-. \tag{2.11}$$

Applying the Lax–Milgram Lemma ([24, Theorem 8.3.4]), we see that the problem (2.8) has a unique solution. Moreover, the variational principle for (2.8) is

$$\inf_{v\in V} E(v), \tag{2.12}$$

where

$$\begin{aligned} E(v) := & \int_{X\times\Omega} \left[\frac{1}{2}\, \Sigma^{-1}(\boldsymbol{\omega}\cdot\nabla v)\, \boldsymbol{\omega}\cdot\nabla v + \frac{1}{2}\, \Sigma(v)\, v - f\, v - \Sigma^{-1}(f)\, \boldsymbol{\omega}\cdot\nabla v \right] \\ & + \int_\Gamma \frac{1}{2}\, |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\, v^2 - 2 \int_{\Gamma_-} |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\, u_{\text{in}} v. \end{aligned}$$

2.2. *Dual formulation*

We next derive a dual formulation for the problem (2.12), following the framework presented in [22]. Let U and P be two normed spaces, U^* and P^* denote their dual spaces. The duality pairings in both U, U^* and P, P^* will be denoted by $\langle \cdot, \cdot \rangle$. Let $\Lambda \in \mathcal{L}(U, P)$. Its transpose $\Lambda^* \in \mathcal{L}(P^*, U^*)$ is defined through the relation

$$\langle \Lambda^* q^*, v \rangle = \langle q^*, \Lambda v \rangle \quad \forall\, v \in U,\ q^* \in P^*.$$

Let J be a functional mapping $U \times P$ into $\overline{\mathbb{R}}$. We consider the minimization problem (the primal problem)

$$\inf_{v\in U} J(v, \Lambda v). \tag{2.13}$$

Its dual problem is defined as

$$\sup_{q^*\in P^*}\left[-J^*(\Lambda^* q^*, -q^*)\right], \tag{2.14}$$

where $J^* : U^* \times P^* \to \overline{\mathbb{R}}$ is the conjugate function of J:

$$J^*(v^*, q^*) = \sup_{\substack{v\in U\\ q\in P}}\left[\langle v^*, v\rangle + \langle q^*, q\rangle - J(v, q)\right], \quad v^* \in U^*,\ q^* \in P^*. \tag{2.15}$$

For the problem (2.12), we choose the space U to be V defined in (1.5) and P to be Q by (1.4). We define the operator Λ by

$$\Lambda v(\boldsymbol{x}, \boldsymbol{\omega}) := \boldsymbol{\omega}\cdot\nabla v(\boldsymbol{x}, \boldsymbol{\omega}). \tag{2.16}$$

Obviously, $\Lambda \in \mathcal{L}(V, Q)$. For a function $v \in V$, we introduce a new variable q for the function $\boldsymbol{\omega}\cdot\nabla v(\boldsymbol{x}, \boldsymbol{\omega})$. Based on the variational formulation (2.12), we introduce the functional

$$\begin{aligned} J(v, q) := &\int_{X\times\Omega}\left[\frac{1}{2}\,\Sigma^{-1}(q)\,q + \frac{1}{2}\,\Sigma(v)\,v - f\,v - \Sigma^{-1}(f)\,q\right] \\ &+ \int_{\Gamma}\frac{1}{2}\,|\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\,v^2 - 2\int_{\Gamma_-}|\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\,u_{\rm in} v. \end{aligned} \tag{2.17}$$

We follow the definition (2.15) to compute

$$J^*(\Lambda^* q^*, -q^*) = \sup_{\substack{v\in V\\ q\in Q}}\left[\langle \Lambda^* q^*, v\rangle - \langle q^*, q\rangle - J(v, q)\right].$$

For $q^* \in V$, we can find that

$$\begin{aligned} J^*(\Lambda^* q^*, -q^*) = &\frac{1}{2}\left(\boldsymbol{\omega}\cdot\nabla q^* - f, \Sigma^{-1}(\boldsymbol{\omega}\cdot\nabla q^* - f)\right)_Q + \frac{1}{2}\left(\Sigma q^* - f, \Sigma^{-1}(\Sigma q^* - f)\right)_Q \\ &+ \frac{1}{2}\,\|q^*\|^2_{\Gamma_+} + \frac{1}{2}\,\|q^* - 2\,u_{\rm in}\|^2_{\Gamma_-}. \end{aligned} \tag{2.18}$$

Consider the dual problem (2.14). Since $C^\infty(\overline{X} \times \Omega)$ is dense in Q, V is also dense in Q. Thus,

$$\sup_{q^*\in Q}\left[-J^*(\Lambda^* q^*, -q^*)\right] = \sup_{q^*\in V}\left[-J^*(\Lambda^* q^*, -q^*)\right].$$

We have, at a maximizer $q^* \in V$, that

$$\begin{aligned} &\left(\Sigma^{-1}(\boldsymbol{\omega}\cdot\nabla q^* - f), \boldsymbol{\omega}\cdot\nabla \delta q^*\right)_Q + \left(\Sigma q^* - f, \delta q^*\right)_Q \\ &+ \left(q^*, \delta q^*\right)_{\Gamma_+} + \left(q^* - 2\,u_{\rm in}, \delta q^*\right)_{\Gamma_-} = 0 \quad \forall\, \delta q^* \in V. \end{aligned} \tag{2.19}$$

Observe that problem (2.19) coincides with the original problem (2.8), i.e. the dual of the problem (2.8) is itself.

3. A posteriori error estimation

In this section, we provide a posteriori error estimates for approximate solutions of the RTE in the energy norm of the space V and in the L^2 norm of Q.

3.1. *A posteriori error estimates in energy norm*

We first recall a basic result in the duality theory; detailed discussion and proofs of these results can be found in [22]. In [23], the duality theory is employed extensively to derive a posteriori estimates for errors of numerical solutions and for errors in mathematical modeling. We use the setting of Subsection 2.2. For the relation between problems (2.13) and (2.14), we have the following duality theorem.

THEOREM 3.1 *Assume the following conditions:*

(1) *U is a reflexive Banach space and P is a normed space; $\Lambda \in \mathcal{L}(U, P)$.*
(2) *$J : U \times P \to \overline{\mathbb{R}}$ is proper, lower semi-continuous, and convex.*
(3) *There exists $u_0 \in U$ such that $J(u_0, \Lambda u_0) < \infty$ and the mapping $q \mapsto J(u_0, q)$ from P to $\overline{\mathbb{R}}$ is continuous at Λu_0.*
(4) *$J(v, \Lambda v) \to +\infty$ as $\|v\| \to \infty$, $v \in U$.*

Then the problem (2.13) has a solution $u \in U$, the problem (2.14) has a solution $p^* \in P^*$, and

$$J(u, \Lambda u) = -J^*(\Lambda^* p^*, -p^*). \tag{3.1}$$

Furthermore, if $J(v, \Lambda v)$ is strictly convex in its effective domain, then a solution u of the problem (2.13) is unique.

We now apply Theorem 3.1 to derive a posteriori error estimates for the RTE problem (1.1)–(1.2). Let w be any given function from V. Consider the quantity

$$D(u, w) := J(w, \Lambda w) - J(u, \Lambda u). \tag{3.2}$$

Using (2.8) with $v = w - u$, we can derive the following formula

$$D(u, w) = \frac{1}{2}\, \|w - u\|_V^2 \tag{3.3}$$

where $\|\cdot\|_V$ is the energy norm over the space V defined in (2.5).

Applying Theorem 3.1, we have

$$D(u, w) \le J(w, \Lambda w) + J^*(\Lambda^* q^*, -q^*) \quad \forall q^* \in V. \tag{3.4}$$

Through algebraic manipulations, we find that

$$\begin{aligned} J(w, \Lambda w) + J^*(\Lambda^* q^*, -q^*) = {} & \frac{1}{2}\int_{X\times\Omega} \Sigma^{-1}(\boldsymbol{\omega}\cdot\nabla w + \Sigma w - f)\,(\boldsymbol{\omega}\cdot\nabla w + \Sigma w - f) \\ & + \frac{1}{2}\int_{X\times\Omega} \Sigma^{-1}\big(\boldsymbol{\omega}\cdot\nabla q^* + \Sigma q^* - f\big)\,\big(\boldsymbol{\omega}\cdot\nabla q^* + \Sigma q^* - f\big) \\ & + \int_{\Gamma_-} |\boldsymbol{\omega}\cdot\boldsymbol{\nu}| \Big[(w - u_{\rm in})^2 + (q^* - u_{\rm in})^2\Big]. \end{aligned}$$

Therefore, we have the following a posteriori error estimate for any $q^* \in V$:

$$\|w-u\|_V^2 \le \left\|\Sigma^{-1/2}(\boldsymbol{\omega}\cdot\nabla w+\Sigma w-f)\right\|_Q^2+2\,\|w-u_{\rm in}\|_{\Gamma_-}^2 \\ +\left\|\Sigma^{-1/2}\big(\boldsymbol{\omega}\cdot\nabla q^*+\Sigma q^*-f\big)\right\|_Q^2+2\,\|q^*-u_{\rm in}\|_{\Gamma_-}^2. \qquad (3.5)$$

The function q^* should be chosen as closely as possible to the solution of the dual problem (2.14), equivalently, that of the original problem (2.8) (cf. (2.19)). When w is the only approximation of u available, it is natural to choose $q^* = w$. With $q^* = w$ in (3.5), we have

$$\|w-u\|_V^2 \le 2\left\|\Sigma^{-1/2}(\boldsymbol{\omega}\cdot\nabla w+\Sigma w-f)\right\|_Q^2+4\,\|w-u_{\rm in}\|_{\Gamma_-}^2. \qquad (3.6)$$

In other words, an a posteriori error bound for $\|u-w\|_V$ is given in terms of the equation residual and boundary condition residual of w.

If $w \in V$ is an approximation of the solution u, then (3.6) provides an a posteriori error bound for the approximate solution. The approximate solution can be computed from a numerical method. If a conforming finite element method is applied to solve (2.8), then the finite element solution $u^h(\boldsymbol{x},\boldsymbol{\omega})$ can be used as the approximate solution of u. An example of a conforming finite element method is the projection of the problem (2.8) onto a conforming finite element space V^h, consisting of functions that are piecewise constant in the variable $\boldsymbol{\omega}$ and are continuous piecewise linear in the variable $\boldsymbol{x}$, corresponding to a finite element partition of the domain $\overline{X}\times\Omega$. The a posteriori error bound (3.6) applies with $w = u^h$.

The angular variable $\boldsymbol{\omega}$ is usually discretized through a discrete-ordinate procedure: the unit sphere Ω is split into a finite number of connected sub-regions: $\Omega = \cup_{l=1}^L \Omega_l$, a representative value $\boldsymbol{\omega}_l$ is selected from Ω_l, and the integral over Ω in the definition of the operator S is approximated by a numerical quadrature with $\{\boldsymbol{\omega}_l\}_{l=1}^L$ as the nodes. The RTE problem (1.1)–(1.2) is then reduced to a system of first-order equations in $\boldsymbol{x}$ along the directions $\{\boldsymbol{\omega}_l\}_{l=1}^L$. Denote by $u_l^h(\boldsymbol{x})$ a finite element approximation of the solution $u(\boldsymbol{x},\boldsymbol{\omega}_l)$ along the direction $\boldsymbol{\omega}_l$. If the finite element space used to compute $\{u_l^h(\boldsymbol{x})\}_{l=1}^L$ consists of continuous piecewise polynomials, then

$$u^h(\boldsymbol{x},\boldsymbol{\omega}) = \sum_{l=1}^L \chi_l(\boldsymbol{\omega})\,u_l^h(\boldsymbol{x}) \qquad (3.7)$$

belongs to V and can be used as an approximate solution for which, the a posteriori error bound (3.6) applies. Here, $\chi_l(\boldsymbol{\omega})$ is the characteristic function of the sub-region Ω_l, i.e. the value of the function is 1 or 0, depending on whether the variable $\boldsymbol{\omega}$ is in or outside Ω_l. If a discontinuous Galerkin finite element method is used to compute $u_l^h(\boldsymbol{x})$, as is the case discussed in [25], then the function u^h defined by (3.7) does not belong to V and (3.6) does not apply directly. In this case, we define a new approximation

$$\bar{u}^h(\boldsymbol{x},\boldsymbol{\omega}) = \sum_{l=1}^L \chi_l(\boldsymbol{\omega})\,\bar{u}_l^h(\boldsymbol{x}), \qquad (3.8)$$

where $\bar{u}_l^h(\boldsymbol{x})$ is constructed from $u_l^h(\boldsymbol{x})$ through an averaging procedure so as to ensure $\bar{u}_l^h(\boldsymbol{x})$ is continuous on X. For simplicity in exposition, suppose $\{u_l^h(\boldsymbol{x})\}_{l=1}^L$ are linear discontinuous Galerkin finite element solutions. Then, at each finite element node $\boldsymbol{x}_i$, we compute a weighted average of the values of $u_l^h(\boldsymbol{x}_i)$ from all elements sharing the node $\boldsymbol{x}_i$, and use the averaging values at all nodes to construct a piecewise linear interpolant $\bar{u}_l^h(\boldsymbol{x})$. The functions $\{\bar{u}_l^h(\boldsymbol{x})\}_{l=1}^L$ are continuous on X. The approximation $\bar{u}^h$ defined in (3.8) belongs to V, and hence the a posteriori error bound (3.6) applies on $\|\bar{u}^h - u\|_V^2$.

Remark 3.2 The inequality (3.6) provides a robust upper bound for the error. A salient feature of the error bound is completely computable. We comment that the error bound is also efficient. To see this, we note that the error function $e := w - u$ is a solution of following problem

$$\boldsymbol{\omega}\cdot\nabla e + \mu_t e - Se = \boldsymbol{\omega}\cdot\nabla w + \Sigma w - f \quad \text{in } X \times \Omega,$$
$$e = w - u_{\text{in}} \quad \text{on } \Gamma_-.$$

By [19, Theorem 3.3], there exists a constant $c_1 \in (0, \infty)$ such that

$$\|\boldsymbol{\omega}\cdot\nabla e\|_Q^2 + \|e\|_Q^2 \ge c_1 \left[\|\boldsymbol{\omega}\cdot\nabla w + \Sigma w - f\|_Q^2 + \|w - u_{\text{in}}\|_{\Gamma_-,*}^2\right],$$

where $\|\cdot\|_{\Gamma_-,*}$ is an L^2-like norm on Γ_-, which is weaker than the norm $\|\cdot\|_{\Gamma_-}$. Using the properties of the operator Σ from Lemma 2.1, we deduce from the above inequality that there exists a constant $c > 0$ such that

$$\|w - u\|_V^2 \ge c \left[\left\|\Sigma^{-1/2}(\boldsymbol{\omega}\cdot\nabla w + \Sigma w - f)\right\|_Q^2 + \|w - u_{\text{in}}\|_{\Gamma_-}^2\right].$$

This shows the efficiency of the error estimate (3.6). Note that, however, it is not easy to provide a reasonably good, explicit numerical value for the constant c.

Next, we derive an a posteriori bound for the error due to noise in data. Let $u^\delta \in V$ be the solution of a perturbed problem:

$$\boldsymbol{\omega}\cdot\nabla u^\delta + \mu_t^\delta u^\delta - S^\delta u^\delta = f^\delta \quad \text{in } X \times \Omega, \tag{3.9}$$
$$u^\delta = u_{\text{in}}^\delta \quad \text{on } \Gamma_-, \tag{3.10}$$

where

$$S^\delta u(\boldsymbol{x}, \boldsymbol{\omega}) = \int_\Omega \mu_s^\delta(\boldsymbol{x}, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\, u(\boldsymbol{x}, \hat{\boldsymbol{\omega}})\, d\hat{\boldsymbol{\omega}}. \tag{3.11}$$

Assume μ_t^δ and μ_s^δ satisfy (1.6) and (1.8), f^δ and u_{in}^δ satisfy (1.9). We apply the bound (3.6) with $w = u^\delta$. Notice that

$$\left\|\Sigma^{-1/2}\big(\boldsymbol{\omega}\cdot\nabla u^\delta + \Sigma u^\delta - f\big)\right\|_Q^2 \le \frac{1}{(1-\kappa)\,\mu_0}\, \|\boldsymbol{\omega}\cdot\nabla u^\delta + \Sigma u^\delta - f\|_Q^2,$$

where (2.2) was used in the last step. So

$$\left\|\Sigma^{-1/2}\big(\boldsymbol{\omega}\cdot\nabla u^\delta + \Sigma u^\delta - f\big)\right\|_Q^2 \le \frac{1}{(1-\kappa)\,\mu_0}\, \left\|\big(\Sigma - \Sigma^\delta\big)(u^\delta) + (f^\delta - f)\right\|_Q^2. \tag{3.12}$$

Define $\Sigma^\delta v := \mu_t^\delta v - S^\delta v$. Then,

$$\boldsymbol{\omega}\cdot\nabla u^\delta + \Sigma u^\delta - f = \big(\Sigma - \Sigma^\delta\big)(u^\delta) + (f^\delta - f)$$

in which

$$\big(\Sigma - \Sigma^\delta\big)(u^\delta) = \big(\mu_t - \mu_t^\delta\big)u^\delta - \int_\Omega \big[\mu_s(\boldsymbol{x}, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}}) - \mu_s^\delta(\boldsymbol{x}, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\big]\, u^\delta(\boldsymbol{x}, \hat{\boldsymbol{\omega}})\, d\hat{\boldsymbol{\omega}}.$$

Thus,

$$\begin{aligned} &\big\|\big(\Sigma - \Sigma^\delta\big)(u^\delta) + (f^\delta - f)\big\|_Q \\ &\quad\le \big\|\big(\mu_t - \mu_t^\delta\big)u^\delta\big\|_Q + \Big\|\int_\Omega \big[\mu_s(\cdot, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}}) - \mu_s^\delta(\cdot, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\big]\, u^\delta(\cdot, \hat{\boldsymbol{\omega}})\, d\hat{\boldsymbol{\omega}}\Big\|_Q \\ &\qquad + \big\|f^\delta - f\big\|_Q. \end{aligned} \tag{3.13}$$

Let

$$\delta_t := \|\mu_t - \mu_t^\delta\|_{L^\infty(X)}, \quad \delta_s := \Big\|\int_\Omega \big|\mu_s(\boldsymbol{x}, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}}) - \mu_s^\delta(\boldsymbol{x}, \boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\big|\, d\hat{\boldsymbol{\omega}}\Big\|_{L^\infty(X)}, \tag{3.14}$$

$$\delta_f := \|f - f^\delta\|_Q, \quad \delta_{\rm in} := \|u_{\rm in} - u_{\rm in}^\delta\|_{L^2(\Gamma_-)}. \tag{3.15}$$

Then, it follows from (3.13) that

$$\big\|\big(\Sigma - \Sigma^\delta\big)(u^\delta) + (f^\delta - f)\big\|_Q \le (\delta_t + \delta_s)\, \|u^\delta\|_Q + \delta_f.$$

Therefore, from (3.6), we conclude the a posteriori error bound

$$\|u - u^\delta\|_V^2 \le \frac{2}{(1-\kappa)\,\mu_0}\, \big[(\delta_t + \delta_s)\, \|u^\delta\|_Q + \delta_f\big]^2 + 4\,\delta_{\rm in}^2. \tag{3.16}$$

In practice, available data contain noises and the RTE problem we solve is not (1.1) and (1.2), but rather (3.9) and (3.10). The significance of the error bound (3.16) is that once the solution u^δ of the problem (3.9)–(3.10) is found, it can be used, together with knowledge of levels of the noises, to generate a computable bound for the difference between u^δ and the solution of the original problem defined by (1.1) and (1.2).

The error bound (3.16) can be sharpened when certain additional information is available. For example, suppose μ_t and μ_t^δ are equal on a portion of the spatial domain X, and so are μ_s and μ_s^δ, i.e.

$$\mu_t^\delta = \mu_t \text{ in } X/X_t, \qquad \mu_s^\delta = \mu_s \text{ in } X/X_s.$$

Then (3.16) can be replaced by

$$\|u - u^\delta\|_V^2 \le \frac{2}{(1-\kappa)\,\mu_0}\, \big[\delta_t \|u^\delta\|_{L^2(X_t\times\Omega)} + \delta_s \|u^\delta\|_{L^2(X_s\times\Omega)} + \delta_f\big]^2 + 4\,\delta_{\rm in}^2. \tag{3.17}$$

3.2. *A posteriori error estimates in L^2 norm*

The L^2 norm error estimates can be derived directly. For an approximate solution $w \in V$ of the problem (1.1)–(1.2), the error $e := w - u$ is the solution of the problem

$$\boldsymbol{\omega}\cdot\nabla e + \mu_t e - S e = e_f \quad \text{in } X \times \Omega, \tag{3.18}$$

$$e = e_{\rm in} \quad \text{on } \Gamma_-, \tag{3.19}$$

where

$$e_f := \boldsymbol{\omega}\cdot\nabla w + \mu_t w - Sw - f \quad \text{in } X \times \Omega, \tag{3.20}$$

$$e_{\text{in}} := w - u_{\text{in}} \quad \text{on } \Gamma_- \tag{3.21}$$

are the residuals of the Equation (1.1) and of the boundary condition (1.2). We multiply the Equation (3.18) by e, integrate over $X \times \Omega$, and perform an integration by parts to obtain

$$\frac{1}{2}\,\|e\|^2_{\Gamma_+} + \left\|\Sigma^{1/2} e\right\|^2_Q = \left(e_f, e\right)_Q + \frac{1}{2}\,\|e_{\text{in}}\|^2_{\Gamma_-}.$$

Using the Cauchy–Schwarz inequality, we conclude with the following a posteriori error estimate:

$$\left\|\Sigma^{1/2}(w-u)\right\|^2_Q + \|w-u\|^2_{\Gamma_+} \le \left\|\Sigma^{-1/2} e_f\right\|^2_Q + \|e_{\text{in}}\|^2_{\Gamma_-}, \tag{3.22}$$

where e_f and e_{in} are defined by (3.20) and (3.21), respectively. This error estimate extends the result in [26], which deals with the homogeneous inflow boundary condition, i.e. $u_{\text{in}} = 0$, and where the approximate solution w is also assumed to satisfy the homogeneous inflow boundary condition.

Next, we consider the error due to perturbations in the problem data, i.e. the difference $e^\delta := u^\delta - u$ between the solutions of the problems (3.9)–(3.10) and (1.1)–(1.2). After subtraction, we see that e^δ satisfies

$$\boldsymbol{\omega}\cdot\nabla e^\delta + \mu_t e^\delta - S e^\delta = e^\delta_f \quad \text{in } X \times \Omega, \tag{3.23}$$

$$e^\delta = e^\delta_{\text{in}} \quad \text{on } \Gamma_-, \tag{3.24}$$

where

$$e^\delta_f := \left(f^\delta - f\right) - \left(\mu^\delta_t - \mu_t\right) u^\delta + \left(S^\delta - S\right) u^\delta \quad \text{in } X \times \Omega, \tag{3.25}$$

$$e^\delta_{\text{in}} := u^\delta_{\text{in}} - u_{\text{in}} \quad \text{on } \Gamma_-. \tag{3.26}$$

Applying the error bound (3.22), we have

$$\left\|\Sigma^{1/2}(u^\delta - u)\right\|^2_Q + \|u^\delta - u\|^2_{\Gamma_+} \le \left\|\Sigma^{-1/2} e^\delta_f\right\|^2_Q + \|e^\delta_{\text{in}}\|^2_{\Gamma_-}. \tag{3.27}$$

Then, with the quantities defined in (3.14) and (3.15), using the bound (2.2), we can obtain from (3.27) that

$$\left\|\Sigma^{1/2}(u^\delta - u)\right\|^2_Q + \|u^\delta - u\|^2_{\Gamma_+} \le \frac{1}{(1-\kappa)\,\mu_0}\left[(\delta_t + \delta_s)\,\|u^\delta\|_Q + \delta_f\right]^2 + \delta^2_{\text{in}}. \tag{3.28}$$

4. Even-parity and odd-parity problems

Let Y be a subset of $X \times \Omega$, or of Γ, or of Ω. We say Y is $\boldsymbol{\omega}$-symmetric if $(\boldsymbol{x}, \boldsymbol{\omega}) \in Y$ implies $(\boldsymbol{x}, -\boldsymbol{\omega}) \in Y$, or if $\boldsymbol{\omega} \in Y$ implies $-\boldsymbol{\omega} \in Y$. Obviously, $X \times \Omega$, Γ, and Ω are $\boldsymbol{\omega}$-symmetric. In the rest of the paper, the symbol Y always denotes a set with $\boldsymbol{\omega}$-symmetry. We say a function $v(\boldsymbol{x}, \boldsymbol{\omega})$ defined on Y is of even parity if $v(\boldsymbol{x}, -\boldsymbol{\omega}) = v(\boldsymbol{x}, \boldsymbol{\omega})$ on Y, and is of odd parity if $v(\boldsymbol{x}, -\boldsymbol{\omega}) = -v(\boldsymbol{x}, \boldsymbol{\omega})$ on Y; where Y is a subset of Ω, we suppress the variable $\boldsymbol{x}$ in the above definition. The following orthogonality property will be used repeatedly:

$$\int_Y u\,v = 0, \quad u \text{ of even-parity and } v \text{ of odd-parity}. \tag{4.1}$$

Even-parity and odd-parity components of $u(\boldsymbol{x},\boldsymbol{\omega})$ were first introduced in [17]:

$$u_+(\boldsymbol{x},\boldsymbol{\omega}) = \frac{1}{2}\left[u(\boldsymbol{x},\boldsymbol{\omega}) + u(\boldsymbol{x},-\boldsymbol{\omega})\right], \quad u_-(\boldsymbol{x},\boldsymbol{\omega}) = \frac{1}{2}\left[u(\boldsymbol{x},\boldsymbol{\omega}) - u(\boldsymbol{x},-\boldsymbol{\omega})\right].$$

They are also called the even-parity angular flux and odd-parity angular flux. The inverse transformation is

$$u(\boldsymbol{x},\boldsymbol{\omega}) = u_+(\boldsymbol{x},\boldsymbol{\omega}) + u_-(\boldsymbol{x},\boldsymbol{\omega}), \quad u(\boldsymbol{x},-\boldsymbol{\omega}) = u_+(\boldsymbol{x},\boldsymbol{\omega}) - u_-(\boldsymbol{x},\boldsymbol{\omega}). \tag{4.2}$$

The parity components of the angular flux $u(\boldsymbol{x},\boldsymbol{\omega})$ are useful in certain applications. E.g. if the goal of computation is to determine the flux $w(\boldsymbol{x}) := \int_\Omega u(\boldsymbol{x},\boldsymbol{\omega})$, then it can also be computed through $w(\boldsymbol{x}) = \int_\Omega u_+(\boldsymbol{x},\boldsymbol{\omega})$. Note that it is less expensive to compute u_+ than u, since $u_+(\boldsymbol{x},\boldsymbol{\omega})$ is even with respect to $\boldsymbol{\omega}$.

Similar to (4.2), we have the decomposition

$$\mu_s(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}}) = \mu_{s+}(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}}) + \mu_{s-}(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})$$

with

$$\mu_{s+}(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}}) = \frac{1}{2}\left[\mu_s(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}}) + \mu_s(\boldsymbol{x},-\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\right],$$
$$\mu_{s-}(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}}) = \frac{1}{2}\left[\mu_s(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}}) - \mu_s(\boldsymbol{x},-\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\right].$$

We introduce two operators C and G^{-1} as follows [21]:

$$C(u_+)(\boldsymbol{x},\boldsymbol{\omega}) := \mu_t(\boldsymbol{x})\,u_+(\boldsymbol{x},\boldsymbol{\omega}) - \int_\Omega \mu_{s+}(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\,u_+(\boldsymbol{x},\hat{\boldsymbol{\omega}})\,d\hat{\boldsymbol{\omega}}, \tag{4.3}$$
$$G^{-1}(u_-)(\boldsymbol{x},\boldsymbol{\omega}) := \mu_t(\boldsymbol{x})\,u_-(\boldsymbol{x},\boldsymbol{\omega}) - \int_\Omega \mu_{s-}(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\,u_-(\boldsymbol{x},\hat{\boldsymbol{\omega}})\,d\hat{\boldsymbol{\omega}}. \tag{4.4}$$

As will be seen from Lemma 4.1 below, the operator defined by the right side of (4.4) is invertible and in the literature, it is denoted by G^{-1}. C is called the removal operator, and G is called the leakage operator. Then, the following result can be shown.

Lemma 4.1 *Assume (1.6) and (1.8). Then, $C : Q_+ \to Q_+$ has an inverse $C^{-1} : Q_+ \to Q_+$, and $G^{-1} : Q_- \to Q_-$ has an inverse $G : Q_- \to Q_-$. Moreover, both C and C^{-1} are linear, bounded, self-adjoint, and elliptic operators on Q_+; both G^{-1} and G are linear, bounded, self-adjoint, and elliptic operators on Q_-.*

Through a formal calculation, the following formulas for C^{-1} and G can be derived [21]:

$$C^{-1}(u_+)(\boldsymbol{x},\boldsymbol{\omega}) = \mu_t(\boldsymbol{x})^{-1}u_+(\boldsymbol{x},\boldsymbol{\omega}) + \int_\Omega k_+(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\,u_+(\boldsymbol{x},\hat{\boldsymbol{\omega}})\,d\hat{\boldsymbol{\omega}}, \tag{4.5}$$
$$G(u_-)(\boldsymbol{x},\boldsymbol{\omega}) = \mu_t(\boldsymbol{x})^{-1}u_-(\boldsymbol{x},\boldsymbol{\omega}) + \int_\Omega k_-(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\,u_-(\boldsymbol{x},\hat{\boldsymbol{\omega}})\,d\hat{\boldsymbol{\omega}}, \tag{4.6}$$

where k_+ and k_- are the even-parity and odd-parity components of k, and k is defined by the equation

$$k(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}}) = \mu_t(\boldsymbol{x})^{-2}\mu_s(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}}) + \mu_t(\boldsymbol{x})^{-1}\int_\Omega \mu_s(\boldsymbol{x},\boldsymbol{\omega}\cdot\overline{\boldsymbol{\omega}})\,k(\boldsymbol{x},\hat{\boldsymbol{\omega}}\cdot\overline{\boldsymbol{\omega}})\,d\overline{\boldsymbol{\omega}}. \tag{4.7}$$

The next result can be proved by applying the Banach fixed-point theorem (cf. e.g. [24, Theorem 5.1.3]).

PROPOSITION 4.2 *Under the assumptions* (1.6) *and* (1.8)*, the Equation* (4.7) *has a unique and non-negative solution* $k(\boldsymbol{x}, \boldsymbol{\omega}{\cdot}\hat{\boldsymbol{\omega}})$ *in* $L^2(X \times \Omega \times \Omega)$.

It is well known [21] that the first-order transport Equation (1.1) is transformed into a pair of second-order equations,

$$-\boldsymbol{\omega}{\cdot}\nabla G(\boldsymbol{\omega}{\cdot}\nabla u_+) + C(u_+) = f_+ - \boldsymbol{\omega}{\cdot}\nabla G(f_-) \tag{4.8}$$

$$-\boldsymbol{\omega}{\cdot}\nabla C^{-1}(\boldsymbol{\omega}{\cdot}\nabla u_-) + G^{-1}(u_-) = f_- - \boldsymbol{\omega}{\cdot}\nabla C^{-1}(f_+). \tag{4.9}$$

Correspondingly, the boundary conditions for the even-parity Equation (4.8) are

$$u_+(\boldsymbol{x}, \boldsymbol{\omega}) - G(\boldsymbol{\omega}{\cdot}\nabla u_+(\boldsymbol{x}, \boldsymbol{\omega})) = u_{\rm in}(\boldsymbol{x}, \boldsymbol{\omega}) - (Gf_-)(\boldsymbol{x}, \boldsymbol{\omega}) \quad \text{for } (\boldsymbol{x}, \boldsymbol{\omega}) \in \Gamma_-, \tag{4.10}$$

$$u_+(\boldsymbol{x}, \boldsymbol{\omega}) + G(\boldsymbol{\omega}{\cdot}\nabla u_+(\boldsymbol{x}, \boldsymbol{\omega})) = u_{\rm in}(\boldsymbol{x}, -\boldsymbol{\omega}) + (Gf_-)(\boldsymbol{x}, \boldsymbol{\omega}) \quad \text{for } (\boldsymbol{x}, \boldsymbol{\omega}) \in \Gamma_+, \tag{4.11}$$

whereas for the odd-parity Equation (4.9),

$$u_-(\boldsymbol{x}, \boldsymbol{\omega}) - C^{-1}(\boldsymbol{\omega}{\cdot}\nabla u_-(\boldsymbol{x}, \boldsymbol{\omega})) = u_{\rm in}(\boldsymbol{x}, \boldsymbol{\omega}) - C^{-1} f_+(\boldsymbol{x}, \boldsymbol{\omega}) \quad \text{for } (\boldsymbol{x}, \boldsymbol{\omega}) \in \Gamma_-, \tag{4.12}$$

$$u_-(\boldsymbol{x}, \boldsymbol{\omega}) + C^{-1}(\boldsymbol{\omega}{\cdot}\nabla u_-(\boldsymbol{x}, \boldsymbol{\omega})) = -u_{\rm in}(\boldsymbol{x}, -\boldsymbol{\omega}) + C^{-1} f_+(\boldsymbol{x}, \boldsymbol{\omega}) \quad \text{for } (\boldsymbol{x}, \boldsymbol{\omega}) \in \Gamma_+. \tag{4.13}$$

To study the well posedness of the even-parity and odd-parity problems, we need some more function spaces. Let

$$V_+ := \{v \in V \mid v(\boldsymbol{x}, -\boldsymbol{\omega}) = v(\boldsymbol{x}, \boldsymbol{\omega})\ \forall\, \boldsymbol{x} \in X,\ \boldsymbol{\omega} \in \Omega\}, \tag{4.14}$$

$$V_- := \{v \in V \mid v(\boldsymbol{x}, -\boldsymbol{\omega}) = -v(\boldsymbol{x}, \boldsymbol{\omega})\ \forall\, \boldsymbol{x} \in X,\ \boldsymbol{\omega} \in \Omega\}, \tag{4.15}$$

$$Q_+ := \{q \in Q \mid q(\boldsymbol{x}, -\boldsymbol{\omega}) = q(\boldsymbol{x}, \boldsymbol{\omega})\ \forall\, \boldsymbol{x} \in X,\ \boldsymbol{\omega} \in \Omega\}, \tag{4.16}$$

$$Q_- := \{q \in Q \mid q(\boldsymbol{x}, -\boldsymbol{\omega}) = -q(\boldsymbol{x}, \boldsymbol{\omega})\ \forall\, \boldsymbol{x} \in X,\ \boldsymbol{\omega} \in \Omega\}. \tag{4.17}$$

Over the spaces Q_+ and Q_-, we use the inner product and norm of the space Q. We use the following inner products

$$(u, v)_{V_+} := (G(\boldsymbol{\omega}{\cdot}\nabla u), \boldsymbol{\omega}{\cdot}\nabla v)_Q + (C(u), v)_Q + (u, v)_\Gamma,$$

$$(u, v)_{V_-} := \left(C^{-1}(\boldsymbol{\omega}{\cdot}\nabla u), \boldsymbol{\omega}{\cdot}\nabla v\right)_Q + \left(G^{-1}(u), v\right)_Q + (u, v)_\Gamma,$$

and corresponding norms. Thanks to Lemma 4.1, the norm $\|\cdot\|_{V_+}$ is equivalent to the canonical norm of V_+ over V_+, while the norm $\|\cdot\|_{V_-}$ is equivalent to the canonical norm of V_- over V_-.

The weak formulation of the boundary value problem of the even-parity equation, defined by (4.8), (4.10), and (4.11), is

$$u_+ \in V_+, \quad \int_{X\times\Omega} [G(\boldsymbol{\omega}{\cdot}\nabla u_+)\, \boldsymbol{\omega}{\cdot}\nabla v + C(u_+)\, v] + \int_\Gamma |\boldsymbol{\omega}{\cdot}\boldsymbol{\nu}|\, u_+ v = \int_{X\times\Omega} [f_+ v + G(f_-)\, \boldsymbol{\omega}{\cdot}\nabla v] + 2\int_{\Gamma_-} |\boldsymbol{\omega}{\cdot}\boldsymbol{\nu}|\, u_{\rm in} v \quad \forall\, v \in V_+. \tag{4.18}$$

Applying the Lax–Milgram Lemma, we see that problem (4.18) has a unique solution.

The weak formulation of the boundary value problem of the odd-parity equation, defined by (4.9), (4.12), and (4.13), is

$$u_- \in V_-, \quad \int_{X\times\Omega} \left[C^{-1}(\boldsymbol{\omega}\cdot\nabla u_-)\,\boldsymbol{\omega}\cdot\nabla v + G^{-1}(u_-)\,v\right] + \int_\Gamma |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\,u_- v$$
$$= \int_{X\times\Omega} \left[f_- v + C^{-1}(f_+)\,\boldsymbol{\omega}\cdot\nabla v\right] + 2\int_{\Gamma_-} |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\,u_{\rm in} v \quad \forall\, v \in V_-. \tag{4.19}$$

The unique solvability of the weak formulation (4.19) also follows from the Lax–Milgram Lemma.

Actually, the problems for the even-parity and odd-parity components can be derived directly from the weak formulation (2.8) of the RTE problem. The operator Σ can be split into the sum of two parts:

$$\Sigma(u) = C(u_+) + G^{-1}(u_-) \tag{4.20}$$

where the operators C and G^{-1} are defined in (4.3) and (4.4). The following result [21] provides a formula for the inverse of the operator Σ:

LEMMA 4.3

$$\Sigma^{-1}(u) = C^{-1}(u_+) + G(u_-). \tag{4.21}$$

Thanks to Lemma 4.1, real powers of C and G are well defined. Moreover, the formulas (4.20) and (4.21) are extended to the following:

$$\Sigma^r(u) = C^r(u_+) + G^{-r}(u_-), \quad r \in \mathbb{R}. \tag{4.22}$$

A consequence of (4.21) is

$$\Sigma^{-1}(\boldsymbol{\omega}\cdot\nabla u) = C^{-1}(\boldsymbol{\omega}\cdot\nabla u_-) + G(\boldsymbol{\omega}\cdot\nabla u_+). \tag{4.23}$$

Now taking $v \in V_+$ arbitrary in (2.8) and using the formulas (4.20), (4.21), and (4.23), we derive from (2.8) that

$$\int_{X\times\Omega} \left[\left(C^{-1}(\boldsymbol{\omega}\cdot\nabla u_-) + G(\boldsymbol{\omega}\cdot\nabla u_+)\right)\boldsymbol{\omega}\cdot\nabla v + \left(C(u_+) + G^{-1}(u_-)\right) v\right]$$
$$+ \int_\Gamma |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\,(u_+ + u_-)\,v$$
$$= \int_{X\times\Omega} \left[(f_+ + f_-)\,v + \left(C^{-1}(f_+) + G(f_-)\right)\boldsymbol{\omega}\cdot\nabla v\right] + 2\int_{\Gamma_-} |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\,u_{\rm in} v.$$

An integral over Ω is zero if the integrand is a product of an even-parity function and an odd-parity function (cf. (4.1)). Hence, the above relation simplifies to the even-parity component problem (4.18). Similarly, taking $v \in V_-$ arbitrary in (2.8), we obtain the odd-parity component problem (4.19).

5. Even-parity and odd-parity problems as dual to each other

We first derive a dual formulation for the even-parity problem.

To use the framework given in Subsection 2.2, we choose the space U to be V_+ according to (4.15) and choose P to be Q_-. We define the operator $\Lambda = \Lambda_+$ by

$$\Lambda_+ v(\boldsymbol{x}, \boldsymbol{\omega}) := \boldsymbol{\omega} \cdot \nabla v(\boldsymbol{x}, \boldsymbol{\omega}). \tag{5.1}$$

Obviously, $\Lambda_+ \in \mathcal{L}(V_+, Q_-)$. For a function $v \in V_+$, we introduce a new variable $q = q(\boldsymbol{x}, \boldsymbol{\omega})$ for the function $\boldsymbol{\omega} \cdot \nabla v(\boldsymbol{x}, \boldsymbol{\omega})$. Corresponding to boundary value problem of the even-parity equation, (4.8), (4.10), and (4.11), based on the weak formulation (4.18), we introduce the functional

$$J_+(v, q) := \frac{1}{2}(q, Gq)_Q + \frac{1}{2}(v, Cv)_Q + \frac{1}{2}\|v\|_\Gamma^2 - (q, Gf_-)_Q - (v, f_+)_Q - 2(u_{\text{in}}, v)_{\Gamma_-}. \tag{5.2}$$

Let $q^* \in V_-$. We follow the definition (2.15) to find

$$\begin{aligned} J_+^*(\Lambda^* q^*, -q^*) = &\frac{1}{2}\Big(\boldsymbol{\omega}\cdot\nabla q^* - f_+, C^{-1}(\boldsymbol{\omega}\cdot\nabla q^* - f_+)\Big)_Q \\ &+ \frac{1}{2}\Big(G^{-1}q^* - f_-, G(G^{-1}q^* - f_-)\Big)_Q + \|q^* - u_{\text{in}}\|_{\Gamma_-}^2. \end{aligned}$$

Since V_- is dense in Q_-, we consider the dual problem

$$\sup_{q^* \in Q_-}\left[-J_+^*(\Lambda^* q^*, -q^*)\right] = \sup_{q^* \in V_-}\left[-J_+^*(\Lambda^* q^*, -q^*)\right].$$

We have, at a maximizer $q^* \in V_-$, that

$$\begin{aligned} &\Big(C^{-1}(\boldsymbol{\omega}\cdot\nabla q^* - f_+), \boldsymbol{\omega}\cdot\nabla \delta q^*\Big)_Q + \Big(G^{-1}q^* - f_-, \delta q^*\Big)_Q \\ &\quad + 2\left(q^* - u_{\text{in}}, \delta q^*\right)_{\Gamma_-} = 0 \quad \forall\, \delta q^* \in V_-. \end{aligned}$$

This is exactly the weak formulation (4.19) of the boundary value problem for the odd-parity component. So the dual variable for the even-parity component is the odd-parity component, and the dual problem of the even-parity component is the problem for the odd-parity component.

Similarly, it can be shown that the dual problem of the odd-parity component is the problem for the even-parity component.

6. Error estimation for parity solutions

For any $w_+ \in V_+$, we define the quantity

$$D_+(u_+, w_+) := J_+(w_+, \Lambda_+ w_+) - J_+(u_+, \Lambda_+ u_+). \tag{6.1}$$

Using (4.18), we can derive the following formula

$$D_+(u_+, w_+) = \frac{1}{2}\|w_+ - u_+\|_{V_+}^2. \tag{6.2}$$

Applying Theorem 3.1, for any $q^* \in V_-$,

$$D_+(u_+, w_+) \le J_+(w_+, \Lambda_+ w_+) + J_+^*(\Lambda_+^* q^*, -q^*). \tag{6.3}$$

Then, we have the a posteriori error estimate: for any $q^* \in V_-$,

$$\|w_+ - u_+\|_{V+}^2 \le \left\|G^{1/2}(\boldsymbol{\omega}\cdot\nabla w_+ + G^{-1}(q^*) - f_-)\right\|_Q^2 + \left\|C^{-1/2}(\boldsymbol{\omega}\cdot\nabla q^* + C(w_+) - f_+)\right\|_Q^2 + 2\,\|w_+ + q^* - u_{\rm in}\|_{\Gamma_-}^2. \quad (6.4)$$

Let $w_- \in V_-$ be an approximation of u_-. Then, we may take q^* in (6.4) to be w_- and obtain the following a posteriori error estimate:

$$\|w_+ - u_+\|_{V+}^2 \le \left\|G^{1/2}(\boldsymbol{\omega}\cdot\nabla w_+ + G^{-1}(w_-) - f_-)\right\|_Q^2 + \left\|C^{-1/2}(\boldsymbol{\omega}\cdot\nabla w_- + C(w_+) - f_+)\right\|_Q^2 + 2\,\|w_+ + w_- - u_{\rm in}\|_{\Gamma_-}^2. \quad (6.5)$$

Note that the RTE (1.1) can be written as

$$\boldsymbol{\omega}\cdot\nabla u_+ + \boldsymbol{\omega}\cdot\nabla u_- + C(u_+) + G^{-1}(u_-) = f_+ + f_- \quad \text{in } X \times \Omega.$$

Taking the even-parity part and odd-parity part of the equation, we obtain

$$\boldsymbol{\omega}\cdot\nabla u_- + C(u_+) = f_+ \quad \text{in } X \times \Omega \quad (6.6)$$

and

$$\boldsymbol{\omega}\cdot\nabla u_+ + G^{-1}(u_-) = f_- \quad \text{in } X \times \Omega, \quad (6.7)$$

respectively. So the first two terms on the right side of (6.5) represent effects of the equation residuals for (6.6) and (6.7). The last term on the right side of (6.5) is for the residual of the boundary condition (1.2).

Based on the duality for the odd-parity solution, we can similarly derive the following a posteriori error estimate:

$$\|w_- - u_-\|_{V-}^2 \le \left\|G^{1/2}(\boldsymbol{\omega}\cdot\nabla w_+ + G^{-1}(w_-) - f_-)\right\|_Q^2 + \left\|C^{-1/2}(\boldsymbol{\omega}\cdot\nabla w_- + C(w_+) - f_+)\right\|_Q^2 + 2\,\|w_+ + w_- - u_{\rm in}\|_{\Gamma_-}^2. \quad (6.8)$$

The bounds (6.5) and (6.8) for the parity solutions together imply (3.6) for the original RTE solution. This claim is based on the relation $\|v\|_V^2 = \|v_+\|_{V+}^2 + \|v_-\|_{V-}^2$ and

$$\left\|\Sigma^{-1/2}(\boldsymbol{\omega}\cdot\nabla v + \Sigma(v) - f)\right\|_Q^2 = \left\|C^{-1/2}(\boldsymbol{\omega}\cdot\nabla v_- + C(v_+) - f_+)\right\|_Q^2 + \left\|G^{1/2}(\boldsymbol{\omega}\cdot\nabla v_+ + G^{-1}(v_-) - f_-)\right\|_Q^2.$$

7. Concluding remarks

This paper is devoted to a concise presentation of rigorous mathematical results on the RTE, and to the development of a posteriori error estimates for numerical solutions of the RTE, as well as for the effects of uncertainties in the problem data on the solution. The boundary value problem of the RTE with the incoming flow boundary condition is adopted as the model for the presentation. It is shown that the boundary value problem of the RTE enjoys beautiful mathematical structures, e.g. the dual of the problem is the problem itself, and the even-parity problem and the odd-parity problem are dual to each other. A posteriori error estimates for numerical solutions are the basis for developing efficient adaptive solution algorithms,[27] whereas a posteriori estimates for modeling errors are useful to analyze the effects of uncertainties in problem data on the solution.[23] Development of adaptive numerical solution algorithms based on the a posteriori error estimates is under the way.

In the previous sections, the theoretical studies are made on the RTE (1.1) with the boundary condition (1.2). We comment that the discussions can be extended to problems with other kind of boundary conditions.

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