SpezialForschungsBereich F 32

Karl–Franzens Universität Graz
Technische Universität Graz
Medizinische Universität Graz

A MIXED VARIATIONAL FRAMEWORK FOR THE RADIATIVE TRANSFER EQUATION

H. Egger M. Schlottbom

SFB-Report No. 2010–40 Dezember 2010

A–8010 GRAZ, HEINRICHSTRASSE 36, AUSTRIA

Supported by the
Austrian Science Fund (FWF)

Der Wissenschaftsfonds.

SFB sponsors:

- **Austrian Science Fund** (FWF)
- **University of Graz**
- **Graz University of Technology**
- **Medical University of Graz**
- **Government of Styria**
- **City of Graz**

A MIXED VARIATIONAL FRAMEWORK FOR THE RADIATIVE TRANSFER EQUATION

HERBERT EGGER AND MATTHIAS SCHLOTTBOM

Abstract. We present a rigorous variational framework for the analysis and discretization of the radiative transfer equation. Existence and uniqueness of weak solutions is established under rather general assumptions on the coefficients. Moreover, weak solutions are shown to be regular and hence also strong solutions of the radiative transfer equation. The relation of the proposed variational method to other approaches, including least-squares and even-parity formulations, is discussed. Moreover, the approximation by Galerkin methods is investigated, and simple conditions are given, under which stable quasi-optimal discretizations can be obtained. For illustration, the approximation by a finite element P_N approximation is discussed in some detail.

1. Introduction

The radiative transfer equation is a basic model for the transport of non-interacting particles with various applications ranging from astrophysics, over neutron transport, to medical imaging. In this paper, we consider stationary monochromatic radiative transfer [12, 10, 9], governed by

$$s\cdot\nabla\phi(r,s) + \mu_t(r)\phi(r,s) = \mu_s(r)\int_{\mathcal{S}} \theta(s\cdot s')\phi(r,s')\,\mathrm{d}s' + q(r,s), \tag{1.1}$$

which characterizes the equilibrium distribution ϕ of a density of particles of fixed energy depending on spatial and angular coordinates r and s, respectively. The first term in the equation models the free transport of particles in direction s, while the second term denotes the absorption of particles by the background medium. The integral term on the right hand side represents the re-emisson of particles after scattering from direction s' into direction s, and q is a source term. We will consider the radiative transfer equation (1.1) in a bounded domain $(r,s)\in\mathcal{D}$, in which case additional boundary conditions have to be prescribed. For our analysis, we utilize the condition

$$\phi = g \quad \text{on } \partial\mathcal{D}_-, \tag{1.2}$$

which allows particles to enter the domain over the inflow part of the boundary. Due to the hyperbolic nature of the equation, no condition can be imposed on the complementing outflow part.

Because of its many applications, the radiative transfer equation (1.1), which is a linearized form of the Boltzmann equation, has been investigated intensively in the past. For instance, in [8], existence of solutions for the transient and stationary case was shown by transforming the integro-differential equation (1.1) into an integral equation, and by the use of Neumann series. A rather complete analytical treatment of the radiative transfer equation based on semi-group theory is given in [11].

Since in complex geometries, (1.1) can hardly be solved analytically, there has been strong interest in the development and analysis of numerical schemes for approximating the solution of the radiative transfer equation. Various methods based on different approximations of the velocity space (e.g., the P_N or S_N approximations), and using different spatial discretizations (e.g. finite difference or finite element methods) have been proposed and investigated in literature. Let us

2000 *Mathematics Subject Classification.* 65N12, 65N30, 35R09.

Key words and phrases. linear Boltzmann equation, neutron transport equation, radiative transfer equation, mixed methods, stable Galerkin approximation, P_N approximation.

refer to [9, 18, 1, 2] for an overview over some approaches and further references.

One of the difficulties in a numerical solution of the radiative transfer equation is its hyperbolic nature, and therefore standard Galerkin discretizations are in general unstable. A possibility to overcome this problem is to transform (1.1) into a second order form, the *even parity formulation*, which is a self-adjoint elliptic problem for only one part of the solution; cf. [12, 18, 1] and the references therein, or Section 5.3. In [19, 20], a different approach, based on a least-squares formulation of the full equation (1.1), has been investigated, which finally also leads to a second order elliptic problem, and admits the stable numerical approximation by Galerkin methods.

In this work, we investigate a new variational approach for the analysis and the numerical solution of (1.1)–(1.2). We consider a weak formulation of the radiative transfer equation in spaces of mixed spatial regularity. This allows us to establish a rigorous variational framework, in which the problem can be shown to be inf-sup stable. Existence and uniqueness of solutions then follow almost automatically from well-known results for linear variational problems and operator equations. We demonstrate, that our variational framework is, in fact, a mixed one, and we establish connections to some other popular formulations of the radiative transfer equation. In particular, we give a rigorous derivation of the even parity formulation within our framework.

The mixed variational framework presented in this paper allows us to apply the Galerkin "machinery", i.e., stable discretizations are obtained by choosing appropriate subspaces of the infinite dimensional spaces and utilizing the same variational principle as on the continuous level. The stability of the resulting discrete problems can be established under simple conditions on the approximations, hence providing quasi-optimal error estimates for a general class of methods. For illustration, we discuss the finite element discretization of a P_N approximation in some detail, and we show that not only odd, but also even order P_N approximations yield stable discretizations, if the correct variational setting is used.

Summarizing, our mixed variational framework allows to treat the analysis and numerical approximation of the radiative transfer equation in a unified systematic manner. Although we only consider the stationary case here, our results will certainly be helpful also for the analysis and discretization of transient problems.

The paper is organized as follows: We start with introducing the relevant notation, and formulate the setting in which we intend to analyze the problem. In Section 3, we then derive a weak form of the radiative transfer equation, we prove the unique solvability, and establish a-priori bounds for the solution. We then show in Section 4, that for sufficiently regular data, any weak solution of the variational problem is, in fact, also a strong solution of the radiative transfer equation. In Section 5, we present some alternative formulations, including a mixed problem, which allows us to give a rigorous derivation of the even parity formulation. We also compare our results to the least-squares formulation of [19]. Section 6 then discusses the approximation of the variational problem by Galerkin methods, and we establish simple sufficient conditions that guarantee the stability of these approximations. For illustration, we also present some details of a coupled finite element P_N approximation, and we close with a short summary.

2. Preliminaries

2.1. **Domains.** Throughout the presentation, we assume that $\mathcal{R} \subset \mathbb{R}^d$, $d = 2, 3$ is a bounded domain with C^1 boundary. By $\mathcal{S} := \{s \in \mathbb{R}^d : |s| = 1\}$, we denote the unit sphere, and we define the product domain $\mathcal{D} := \mathcal{R} \times \mathcal{S}$; cf. Figure 1. Let $n(r)$ be the outward pointing normal vector for a point $r \in \partial\mathcal{R}$. The boundary $\partial\mathcal{D} := \partial\mathcal{R} \times \mathcal{S}$ can be decomposed into an inflow part $\partial\mathcal{D}_- = \{(r, s) \in \partial\mathcal{D} : n \cdot s < 0\}$, an outflow part $\partial\mathcal{D}_+$ where $n \cdot s > 0$, and a remaining tangential part $\partial\mathcal{D}_0$. Due to regularity of the boundary, the normal vector is continuous, and hence $\partial\mathcal{D}_\pm$ are open subsets of $\partial\mathcal{D}$, and $\partial\mathcal{D}_0$ is closed with surface measure zero; cf. Lemma A1. This allows to

identify measurable functions defined on $\partial\mathcal{D}$ with those defined on $\partial\mathcal{D}_- \cup \partial\mathcal{D}_+$. Here and below, the symbol $\pm$ is used to treat the two cases $+$ and $-$ in compact form.

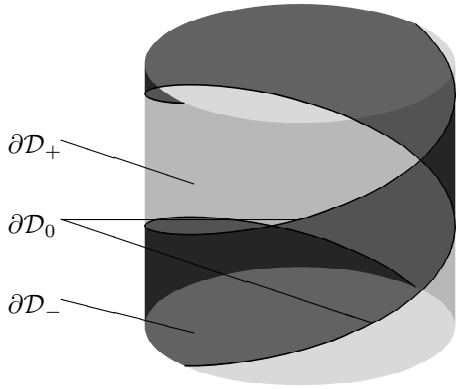

FIGURE 1. Schematic diagram of the domain $\mathcal{D} = \mathcal{R} \times \mathcal{S}$, with $\mathcal{R}$ being the two-dimensional unit circle. The angular domain $\mathcal{S}$ is identified with the interval $[0, 2\pi)$ via $s = (\cos(\alpha), \sin(\alpha))^\top$. The inflow part $\partial\mathcal{D}_-$ is shaded in dark-gray, while the outflow boundary $\partial\mathcal{D}_+$ is in light-gray. The separating black curves denote $\partial\mathcal{D}_0$.

2.2. **Function spaces and traces.** By $\mathbb{V}_0 := L^2(\mathcal{D})$, we denote the Lebesgue space of square integrable functions over $\mathcal{D}$ with scalar product $(v, w)_{\mathbb{V}_0} := (v, w)_{\mathcal{D}}$, where

$$(v, w)_{\mathcal{D}} := \int_{\mathcal{R}} \int_{\mathcal{S}} v(r, s) w(r, s) \, \mathrm{d}s \, \mathrm{d}r.$$

Similar notation is used for scalar products defined as integrals over other domains, and the norm associated with a scalar product $(\cdot, \cdot)_*$ is always denoted by $\|v\|_* := \sqrt{(v, v)_*}$.

Remark 2.1. In our analysis, we only consider the case of real valued fields. If the scalar products are adapted appropriately, e.g. with conjugation of the first argument, all results derived in the following hold, with minor modifications, also for complex valued function spaces. This case arises, e.g., when time harmonic (intensity modulated) fields are considered, see [24, 23], or in the approximation of the radiative transfer equation by spherical harmonics; cf. [12, 9] and Section 6.1.

For smooth functions $v \in C^\infty(\overline{\mathcal{D}})$, we define another scalar product by

$$(v, w)_{\mathbb{V}_1} := (v, w)_{\mathcal{D}} + (s \cdot \nabla v, s \cdot \nabla w)_{\mathcal{D}} + (|n \cdot s| v, w)_{\partial\mathcal{D}},$$

and we denote by $\mathbb{V}_1$ the completion of $C^\infty(\overline{\mathcal{D}})$ with respect to the associated norm. Functions in $\mathbb{V}_1$ have well-defined boundary values (see appendix): Let us denote by $\mathbb{T}$ the completion of $L^2(\partial\mathcal{D})$ with respect to the norm associated with

$$(v, w)_{\mathbb{T}} := (|n \cdot s| \, v, w)_{\partial\mathcal{D}}.$$

The following statement then is a direct consequence of the construction of the spaces $\mathbb{V}_1$ and $\mathbb{T}$.

Lemma 2.2. *The trace mapping $v \mapsto v|_{\partial\mathcal{D}}$ defined for $v \in C^1(\overline{\mathcal{D}})$ can be extended by continuity to a bounded linear operator $\gamma : \mathbb{V}_1 \to \mathbb{T}$ with $\|\gamma(v)\|_{\mathbb{T}} \leq \|v\|_{\mathbb{V}_1}$ for all $v \in \mathbb{V}_1$.*

We denote by $\mathbb{T}_\pm := \{v|_{\partial\mathcal{D}_\pm} : v \in \mathbb{T}\}$ the restriction of functions in $\mathbb{T}$ to the inflow and outflow parts of the boundary. The partial trace maps $\gamma_\pm : \mathbb{V}_1 \to \mathbb{T}_\pm$, $v \mapsto v|_{\partial\mathcal{D}_\pm}$ are again bounded linear operators. In fact $\gamma_\pm$ can be shown to be surjective; cf. Lemma A2.

Remark 2.3. Functions in the space $\widehat{\mathbb{V}}_1 := \{v \in \mathbb{V}_0 : s\cdot\nabla v \in \mathbb{V}_0\}$, which is larger than $\mathbb{V}_1$, already have enough regularity to admit the notion of boundary values [20, 11]. The space $\mathbb{V}_1$ can therefore be characterized alternatively as proper subspace $\mathbb{V}_1 = \{v \in \widehat{\mathbb{V}}_1 : \|\gamma(v)\|_{\mathbb{T}} < \infty\} \subset \widehat{\mathbb{V}}_1$. For further details, we refer to [20] and the appendix.

2.3. **Even–Odd splitting.** The following splitting is a standard tool in the analysis of the radiative transfer equation, cf. [18, 1]. For a measurable function v on $\mathcal{S}$, we define its even (v^+) and odd (v^-) parts by

$$v^\pm(s) := \frac{1}{2}\big(v(s) \pm v(-s)\big). \tag{2.1}$$

A function v is called *even* (to have *even parity*), if $v = v^+$, and *odd* (of *odd parity*), if $v = v^-$. Any function $v \in L^2(\mathcal{S})$ can be split uniquely into its even and odd components, i.e, $v = v^+ + v^-$, and this splitting is orthogonal with respect to the $L^2(\mathcal{S})$ scalar product. In the same way, one can define the splitting of functions, which additionally depend on a spatial variable, i.e. by $v^\pm(r,s) := \frac{1}{2}(v(r,s) \pm v(r,-s))$. We then denote by

$$\mathbb{V}^\pm := \{v^\pm : v \in \mathbb{V}\},$$

the subspaces of even and odd functions of $\mathbb{V}$. The following result is a direct consequence of the definition of the spaces and scalar products in the previous section.

Lemma 2.4. *Any of the spaces $\mathbb{V} \in \{\mathbb{V}_0, \mathbb{V}_1, \mathbb{T}\}$ can be split into $\mathbb{V} = \mathbb{V}^+ \oplus \mathbb{V}^-$, and the splitting is orthogonal with respect to the scalar product of $\mathbb{V}$.*

2.4. **Operators.** In the sequel, we formally introduce the operators appearing in the radiative transfer equation (1.1), and we summarize their basic properties relying on rather general assumptions about the parameters. Most of the following results are well-known, and can be found for instance in [11].

2.4.1. *Transport.* Let us begin with the advection (transport) operator, which is defined as

$$\mathcal{A} : \mathbb{V}_1 \to \mathbb{V}_0, \qquad (\mathcal{A}v)(r,s) := s\cdot\nabla v(r,s).$$

The following basic properties of $\mathcal{A}$ follow almost directly from its definition.

Lemma 2.5. *$\mathcal{A} : \mathbb{V}_1 \to \mathbb{V}_0$ is a bounded linear operator with $\|\mathcal{A}v\|_{\mathbb{V}_0} \le \|v\|_{\mathbb{V}_1}$ for all $v \in \mathbb{V}_1$. Moreover, for any $v^\pm \in \mathbb{V}_1^\pm$ we have $\mathcal{A}v^\pm \in \mathbb{V}_0^\mp$, i.e., $\mathcal{A}$ maps even to odd, and odd to even functions; we say that $\mathcal{A}$ is* parity reversing.

Proof. Boundedness is a direct consequence of the definition of the norms and the operator. The parity reversing property then follows from $(\mathcal{A}v)(-s) = -s\cdot\nabla v(-s)$, and inserting even or odd functions v. □

The following integration-by-parts formula will be a central tool for the derivation of a weak formulation in the next section.

Lemma 2.6. *For any pair of functions v, $w \in \mathbb{V}_1$ there holds*

$$(\mathcal{A}v, w)_{\mathcal{D}} = -(v, \mathcal{A}w)_{\mathcal{D}} + (n\cdot s\, v, w)_{\partial\mathcal{D}}. \tag{2.2}$$

Proof. For smooth functions $v \in \mathcal{C}^\infty(\overline{\mathcal{D}})$, the formula is a direct consequence of Green's theorem, and the result then follows by a density argument. □

Remark 2.7. Lemma 2.6 does not hold for arbitrary functions in the larger space $\widehat{\mathbb{V}}_1$, since the boundary values do not have the required regularity; cf. Lemma A2. One possible generalization of (2.2) for functions in $\widehat{\mathbb{V}}_1$ will be stated in Lemma 4.2.

2.4.2. *Scattering.* The scattering operator Θ, associated with a scattering kernel θ, is defined by

$$\Theta : \mathbb{V}_0 \to \mathbb{V}_0, \qquad (\Theta v)(r,s) := \int_{\mathcal{S}} \theta(r, s\cdot s')v(r,s')ds'.$$

Remark 2.8. To simplify the notation, we will often neglect the spatial dependence and simply write $(\Theta v)(s) = \int_{\mathcal{S}} \theta(s\cdot s')v(s')\,\mathrm{d}s'$, instead.

In the sequel, we assume that the scattering kernel θ satisfies the following conditions.

Assumption 2.9. *(S1) θ is a measurable function and positive, i.e., $\theta(r, s\cdot s') \geq 0$ for a.e. $r \in \mathcal{R}$ and $s, s' \in \mathcal{S}$; (S2) θ is normalized to one, i.e., $\int_{\mathcal{S}} \theta(r, s\cdot s')\,ds' = 1$ for a.e. $(r,s) \in \mathcal{D}$.*

The assumptions on the scattering kernel imply the following properties of the scattering operator.

Lemma 2.10. *$\Theta : \mathbb{V}_0 \to \mathbb{V}_0$ is a self-adjoint and bounded linear operator with $\|\Theta v\|_{\mathbb{V}_0} \leq \|v\|_{\mathbb{V}_0}$ for all $v \in \mathbb{V}_0$. Moreover, $\Theta v^{\pm} \in \mathbb{V}_0^{\pm}$ for any $v \in \mathbb{V}_0$, i.e., the scattering operator is* parity preserving.

Proof. Linearity of Θ is obvious, and self-adjointness follows from the symmetry of $\theta(s\cdot s')$ with respect to s and s'. By normalization and positivity of the kernel, and using the Cauchy-Schwarz inequality, we obtain as in [11, Ch XXI 2.3.1]

$$\begin{aligned}\|\Theta v\|^2_{L^2(\mathcal{S})} &= \int_{\mathcal{S}} \Big| \int_{\mathcal{S}} \theta(s\cdot s')v(s')\,\mathrm{d}s'\Big|^2\,\mathrm{d}s \\ &\leq \int_{\mathcal{S}} \Big(\int_{\mathcal{S}} \theta(s\cdot s')\,\mathrm{d}s'\Big)\Big(\int_{\mathcal{S}} \theta(s\cdot s')|v(s')|^2\,\mathrm{d}s'\Big)\,\mathrm{d}s \\ &= \int_{\mathcal{S}}\int_{\mathcal{S}} \theta(s\cdot s')\,\mathrm{d}s|v(s')|^2\,\mathrm{d}s' = \|v\|^2_{L^2(\mathcal{S})}.\end{aligned}$$

For ease of notation, we suppressed the dependence on the spatial variable r. Integration over $\mathcal{R}$ yields the bound $\|\Theta v\|_{\mathbb{V}_0} \leq \|v\|_{\mathbb{V}_0}$. Note that application of Θ to the constant function $v \equiv 1$ gives $\|\Theta 1\|_{\mathbb{V}_0} = \|1\|_{\mathbb{V}_0}$, so that the bound is optimal. Furthermore, we obtain for every even function $v \in \mathbb{V}_0^+$ that

$$\begin{aligned}(\Theta v)(s) &= \frac{1}{2}\int_{\mathcal{S}} \theta(s\cdot s')(v(s') + v(-s'))\,\mathrm{d}s' \\ &= \frac{1}{2}\int_{\mathcal{S}} \theta(s\cdot s')v(s')\,\mathrm{d}s' + \frac{1}{2}\int_{\mathcal{S}} \theta(-s\cdot s')v(s')\,\mathrm{d}s' = \frac{1}{2}\big[(\Theta v)(s) + (\Theta v)(-s)\big]\end{aligned}$$

which shows that Θv is even, whenever $v \in \mathbb{V}_0^+$. In the same way, one sees that Θv is odd for $v \in \mathbb{V}_0^-$. Hence, the scattering operator is parity preserving. □

Remark 2.11. Since θ is real valued, the properties stated in Lemma 2.10 carry over to the case of complex valued functions with identical proofs.

2.4.3. *Absorption and removal.* It will turn out to be convenient for our analysis, to represent absorption and scattering by a single operator. Given two coefficient functions μ_a and μ_s, we define the *removal operator* [1] by

$$\mathcal{C} : \mathbb{V}_0 \to \mathbb{V}_0, \qquad (\mathcal{C}v)(r,s) := \mu_a(r)v(r,s) + \mu_s(r)\big(v(r,s) - (\Theta v)(r,s)\big).$$

Remark 2.12. The first part $\mu_a(r)v(r,s)$ of the removal operator models the absorption of particles by the medium, while the second part $\mu_s(r)\big(v(r,s) - (\Theta v)(r,s)\big)$ describes the absorption and re-emission of particles during the scattering process. In operator notation, one could also write $\mathcal{C} = \mu_a\mathcal{I} + \mu_s(\mathcal{I} - \Theta)$ with $\mathcal{I}$ denoting the identity operator. In view of (1.1), the total absorption regarding one particular direction s is governed by the parameter $\mu_t = \mu_a + \mu_s$.

In order to derive useful properties of the removal operator, we require that the scattering and absorption parameters μ_s and μ_a satisfy the following conditions.

Assumption 2.13. *(C1) μ_s is measurable, non-negative, and uniformly bounded, i.e., there exists a positive constant $\overline{\mu}_s$ such that $0 \leq \mu_s(r) \leq \overline{\mu}_s$ for a.e. $r \in \mathcal{R}$. (C2) μ_a is measurable, uniformly positive, and bounded, i.e., $0 < \underline{\mu}_a \leq \mu_a(r) \leq \overline{\mu}_a$ for a.e. $r \in \mathcal{R}$ for some $\underline{\mu}_a$, $\overline{\mu}_a > 0$.*

Based on assumptions (C1)–(C2) on the coefficients, the removal operator can be shown to have the following properties; see also [11, Ch XXI 2.4.1 Theorem 4].

Lemma 2.14. *$\mathcal{C} : \mathbb{V}_0 \to \mathbb{V}_0$ is a self-adjoint and elliptic bounded linear operator, i.e.*

$$(\mathcal{C}v, v)_{\mathcal{D}} \geq \underline{\mu}_a \|v\|^2_{\mathbb{V}_0} \qquad \text{and} \qquad \|\mathcal{C}v\|_{\mathbb{V}_0} \leq (2\overline{\mu}_s + \overline{\mu}_a)\|v\|_{\mathbb{V}_0}.$$

Moreover, $\mathcal{C}$ is parity preserving, i.e., $\mathcal{C}v^{\pm} \in \mathbb{V}_0^{\pm}$ for any $v \in \mathbb{V}_0$.

Proof. Linearity and self-adjointness follow directly from the definition and the properties of the scattering operator. By the Cauchy-Schwarz inequality, we obtain (for a.e. $r \in \mathcal{R}$),

$$(v, \Theta v)_{\mathcal{S}} \leq \|\Theta v\|_{L^2(\mathcal{S})}\|v\|_{L^2(\mathcal{S})} \leq \|v\|^2_{L^2(\mathcal{S})},$$

where we used the bound of Lemma 2.10 for the second inequality. Multiplying by μ_s and integrating over $\mathcal{R}$, we obtain that $(\mu_s \Theta v, v)_{\mathcal{D}} \leq (\mu_s v, v)_{\mathcal{D}}$, and consequently

$$(\mathcal{C}v, v)_{\mathcal{D}} = (\mu_a v, v)_{\mathcal{D}} + (\mu_s v, v)_{\mathcal{D}} - (\mu_s \Theta v, v)_{\mathcal{D}} \geq \underline{\mu}_a \|v\|^2_{\mathbb{V}_0}.$$

The upper bound then follows from the corresponding bound for the scattering operator and the triangle inequality. Since Θ and the identity operator are both parity preserving, the same holds true for the removal operator. □

Remark 2.15. If the parameters μ_a and μ_s are real valued, the properties carry over verbatim to the case of a complex valued function space $\mathbb{V}_0$. Time harmonic fields, for which μ_a would be complex, can then be treated similarly, if the real part of μ_a is uniformly bounded from below.

By the Lax-Milgram lemma, and the ellipticity and boundedness of the removal operator, $\mathcal{C}$ is boundedly invertible, and we can define two norms

$$\|v\|^2_{\mathcal{C}^{-1}} := (\mathcal{C}^{-1}v, v)_{\mathcal{D}} \qquad \text{and} \qquad \|v\|^2_{\mathcal{C}} := (\mathcal{C}v, v)_{\mathcal{D}}, \tag{2.3}$$

on $\mathbb{V}_0$, which have the following properties.

Lemma 2.16. *The norms* (2.3) *induced by $\mathcal{C}$ and $\mathcal{C}^{-1}$ are equivalent to the norm of $\mathbb{V}_0$, i.e., for all functions $v \in \mathbb{V}_0$ there holds*

$$c\|v\|^2_{\mathbb{V}_0} \leq \|v\|^2_{\mathcal{C}} \leq C\|v\|^2_{\mathbb{V}_0} \qquad \text{and} \qquad C^{-1}\|v\|^2_{\mathbb{V}_0} \leq \|v\|^2_{\mathcal{C}^{-1}} \leq c^{-1}\|v\|^2_{\mathbb{V}_0}$$

with equivalence constants given by $c = \underline{\mu}_a$ and $C = 2\overline{\mu}_s + \overline{\mu}_a$.

Remark 2.17. If Θ is positive semi-definite, the upper bound can be sharpened to $C = \overline{\mu}_s + \overline{\mu}_a$. This is the case, for instance, if in addition to Assumption 2.9, the scattering is absolutely forward dominant, which is true for isotropic, Rayleigh or Thompson scattering [17]. A refined analysis also allows to relax the conditions on μ_a and μ_s to some extent; cf. [20].

2.5. **Operator formulation.** Using the operators defined in the previous section, the radiative transfer equation (1.1)–(1.2) can now be written in compact form as

$$\mathcal{A}\phi + \mathcal{C}\phi = q \qquad \text{a.e. in } \mathcal{D}, \tag{2.4}$$

$$\gamma_-(\phi) = g \qquad \text{a.e. on } \partial\mathcal{D}_-. \tag{2.5}$$

Definition 2.18. *A function $\phi \in \mathbb{V}_1$, which satisfies* (2.4) *and* (2.5) *for given $q \in L^2(\mathcal{D})$ and $g \in L^2(\partial\mathcal{D}_-)$ is called* strong solution *of the radiative transfer equation.*

As outlined in the introduction, there exist several ways for establishing the existence of solutions to the radiative transfer equation. Our approach, presented in the following two sections, is based on variational arguments.

3. A variational formulation

In this section, we derive a variational formulation of the radiative transfer equation (2.4)–(2.5), which is *weak* in the sense that we require less regularity on the solution than used for the definition of strong solutions. We will prove the existence and uniqueness of a solution to this weak formulation, and show that any weak solution is in fact also a strong solution in the sense of Definition 2.18.

3.1. **Derivation of the variational principle.** Assume that $\phi \in \mathbb{V}_1$ is a strong solution of the radiative transfer equation (2.4)–(2.5). Multiplying (2.4) with a test function $\psi \in \mathbb{V}_1$, and integrating over the domain $\mathcal{D}$, we obtain

$$(\mathcal{A}\phi, \psi)_{\mathcal{D}} + (\mathcal{C}\phi, \psi)_{\mathcal{D}} = (q, \psi)_{\mathcal{D}}. \tag{3.1}$$

Using the unique decomposition of functions into even and odd parts, and the parity reversing property of the operator $\mathcal{A}$, equation (3.1) can be written equivalently as

$$(\mathcal{A}\phi^+, \psi^-)_{\mathcal{D}} + (\mathcal{A}\phi^-, \psi^+)_{\mathcal{D}} + (\mathcal{C}\phi, \psi)_{\mathcal{D}} = (q, \psi)_{\mathcal{D}}. \tag{3.2}$$

By means of the integration-by-parts formula (2.2), the second term can be transformed into

$$(\mathcal{A}\phi^-, \psi^+)_{\mathcal{D}} = -(\phi^-, \mathcal{A}\psi^+)_{\mathcal{D}} + (n\cdot s\ \phi^-, \psi^+)_{\partial\mathcal{D}}. \tag{3.3}$$

Using the boundary condition (2.5), and noting that $s \mapsto n\cdot s\ \phi^-\psi^+$ is an even function, we can further rewrite the boundary term as

$$\begin{aligned}(n\cdot s\ \phi^-, \psi^+)_{\partial\mathcal{D}} &= 2\int_{\partial\mathcal{R}}\int_{n\cdot s<0} n\cdot s\ (g-\phi^+)\psi^+\,\mathrm{d}s\,\mathrm{d}\sigma \\ &= (|n\cdot s|\ \phi^+, \psi^+)_{\partial\mathcal{D}} + 2(n\cdot s\ g, \psi^+)_{\partial\mathcal{D}_-}.\end{aligned} \tag{3.4}$$

The combination of (3.2)–(3.4) then yields the following weak characterization of solutions.

Lemma 3.1. *Any strong solution ϕ of the radiative transfer equation* (2.4)–(2.5) *also satisfies*

$$b(\phi, \psi) = \ell(\psi) \qquad \text{for all } \psi \in \mathbb{V}_1, \tag{3.5}$$

with bilinear form b and linear form ℓ defined by

$$b(\phi, \psi) := (\mathcal{C}\phi, \psi)_{\mathcal{D}} - (\phi^-, \mathcal{A}\psi^+)_{\mathcal{D}} + (\mathcal{A}\phi^+, \psi^-)_{\mathcal{D}} + (|n\cdot s|\ \phi^+, \psi^+)_{\partial\mathcal{D}} \tag{3.6}$$

$$\ell(\psi) := (q, \psi)_{\mathcal{D}} - 2(n\cdot s\ g, \psi^+)_{\partial\mathcal{D}_-}. \tag{3.7}$$

Note that both forms involve only derivatives of the even components ϕ^+ and ψ^+ of the solution and the test function, respectively. This leads us to the definition of the space

$$\mathbb{W} := \mathbb{V}_1^+ \oplus \mathbb{V}_0^- \tag{3.8}$$

which turns out to be the natural *energy* space for our analysis.

Remark 3.2. Only the even components v^+ of functions $v \in \mathbb{W}$ have some spatial regularity, and we therefore refer to $\mathbb{W}$ as space of *mixed regularity*. Also note that $\mathbb{W}^+ = \mathbb{V}_1^+$ and $\mathbb{W}^- = \mathbb{V}_0^-$. Due to the unique splitting of functions into even and odd parts, the space $\mathbb{W} = \mathbb{V}_1^+ \oplus \mathbb{V}_0^-$ can be identified with the product space $\mathbb{V}_1^+ \times \mathbb{V}_0^-$; we will return to this viewpoint in Section 5.2.

The weak form of the radiative transfer equation then leads to the following variational problem.

Problem 1. *Given $q \in L^2(\mathcal{D})$ and $g \in L^2(\partial\mathcal{D}_-)$, find $\phi \in \mathbb{W}$ which satisfies* (3.5).

Definition 3.3. *A solution of Problem 1 is called* weak solution *of the radiative transfer equation.*

The natural norm for the space $\mathbb{W}$ would be the one inherited from the spaces $\mathbb{V}_1^+$ and $\mathbb{V}_0^-$. For the subsequent analysis, it is however convenient to equip $\mathbb{W}$ with a different *energy norm*, viz.

$$\|v\|_{\mathbb{W}} := \big(\|\mathcal{A}v^+\|_{\mathcal{C}^{-1}}^2 + \|v\|_{\mathcal{C}}^2 + \|\gamma(v^+)\|_{\mathbb{T}}^2\big)^{1/2}. \tag{3.9}$$

By application of Lemma 2.16, this norm can be shown to be equivalent to the norm of $\mathbb{V}_1^+ \oplus \mathbb{V}_0^-$.

Lemma 3.4. *Let the assumptions of Lemma 2.16 hold. Then*

$$c\|v\|_{\mathbb{W}}^2 \le \|v^+\|_{\mathbb{V}_1}^2 + \|v^-\|_{\mathbb{V}_0}^2 \le C\|v\|_{\mathbb{W}}^2 \tag{3.10}$$

with equivalence constants $c = \min\{\underline{\mu}_a, 1/(2\overline{\mu}_s + \overline{\mu}_a)\}$ and $C = \max\{2\overline{\mu}_s + \overline{\mu}_a, \underline{\mu}_a^{-1}\}$.

Remark 3.5. The space $\mathbb{W}$ is again a Hilbert space, and the inclusions $\mathbb{V}_1 \subset \mathbb{W} \subset \mathbb{V}_0$ are strict and dense (see appendix). This shows that the variational form (3.5) is in fact weaker than the strong form (2.4)–(2.5) of the radiative transfer equation.

3.2. **Unique solvability.** The aim of this section is to establish the existence of a unique solution to Problem 1. To do so, we require some basic properties of the bilinear and linear forms used in the variational principle (3.5), which we derive in the following.

Proposition 3.6. *The linear form ℓ is bounded on $\mathbb{W}$, i.e., there holds $|\ell(\psi)| \leq C_\ell \|\psi\|_{\mathbb{W}}$ for all $\psi \in \mathbb{W}$, i.e., $\|\ell\|_{\mathbb{W}'} \leq C_l$, with constant $C_\ell = (\sqrt{2}\|g\|^2_{\partial\mathcal{D}_-} + \underline{\mu}_a^{-1}\|q\|^2_{\mathcal{D}})^{1/2}$.*

Proof. By definition of the linear form and the Cauchy-Schwarz inequality, we have

$$\ell(\psi) = (q,\psi)_{\mathcal{D}} + 2(|n\cdot s|\, g, \psi^+)_{\partial\mathcal{D}_-} \leq 2\|g\|_{\partial\mathcal{D}_-}\|\psi^+\|_{\mathbb{T}_-} + \|q\|_{\mathcal{C}^{-1}}\|\psi\|_{\mathcal{C}}.$$

The bound then follows by Lemma 2.16, the fact that $\|\psi^+\|_{\mathbb{T}} = \sqrt{2}\|\psi^+\|_{\mathbb{T}_-}$, which is shown similarly to (3.4), and by another application of the Cauchy-Schwarz inequality. □

Continuity of the bilinear form follows again almost directly from the definition of the norm of $\mathbb{W}$.

Proposition 3.7. *The bilinear form b is bounded on $\mathbb{W}\times\mathbb{W}$ with $|b(\phi,\psi)| \leq 2\|\phi\|_{\mathbb{W}}\|\psi\|_{\mathbb{W}}$.*

Proof. Application of the Cauchy-Schwarz inequality yields

$$b(\phi,\psi) \leq \|\phi\|_{\mathcal{C}}\|\psi\|_{\mathcal{C}} + \|\phi\|_{\mathcal{C}}\|\mathcal{A}\psi^+\|_{\mathcal{C}^{-1}} + \|\mathcal{A}\phi^+\|_{\mathcal{C}^{-1}}\|\psi\|_{\mathcal{C}} + \|\phi^+\|_{\mathbb{T}}\|\psi^+\|_{\mathbb{T}} \leq 2\|\phi\|_{\mathbb{W}}\|\psi\|_{\mathbb{W}},$$

where we used $a_1b_1 + a_1b_2 + a_2b_1 + c_1c_2 \leq (2a_1^2 + a_2^2 + c_1^2)^{1/2}(2b_1^2 + b_2^2 + c_2^2)^{1/2}$ for the second estimate, which again follows from the Cauchy-Schwarz inequality. □

The main property to ensure unique solvability of Problem 1 are the following stability conditions.

Proposition 3.8. *The bilinear form b is* inf-sup *stable on $\mathbb{W}\times\mathbb{W}$, i.e., the two estimates*

$$\sup_{\|\psi\|_{\mathbb{W}}=1} b(\phi,\psi) \geq \beta\|\phi\|_{\mathbb{W}} \qquad \text{and} \qquad \sup_{\|\psi\|_{\mathbb{W}}=1} b(\psi,\phi) \geq \beta\|\phi\|_{\mathbb{W}}$$

hold uniformly for all $\phi \in \mathbb{W}$ with stability constant $\beta := (2\sqrt{3})^{-1}$.

Proof. For $\phi = 0$ the assertion is trivial, so we can assume that $\phi \in \mathbb{W}\setminus\{0\}$. In the following three steps, we explicitly construct a test function $\psi \in \mathbb{W}$ that satisfies the first estimate:
(i) Testing with $\psi := \phi$, we obtain by the symmetry of the inner product that

$$b(\phi,\phi) = \|\phi\|^2_{\mathcal{C}} - (\phi^-, \mathcal{A}\phi^+)_{\mathcal{D}} + (\mathcal{A}\phi^+, \phi^-)_{\mathcal{D}} + \|\phi^+\|^2_{\mathbb{T}} = \|\phi\|^2_{\mathcal{C}} + \|\phi^+\|^2_{\mathbb{T}}.$$

(ii) Testing with $\psi := \mathcal{C}^{-1}\mathcal{A}\phi^+ \in \mathbb{W}^-$ yields

$$\begin{aligned} b(\phi, \mathcal{C}^{-1}\mathcal{A}\phi^+) &= (\mathcal{C}\phi^-, \mathcal{C}^{-1}\mathcal{A}\phi^+)_{\mathcal{D}} + (\mathcal{A}\phi^+, \mathcal{C}^{-1}\mathcal{A}\phi^+)_{\mathcal{D}} \\ &= (\mathcal{C}^{1/2}\phi^-, \mathcal{C}^{-1/2}\mathcal{A}\phi^+)_{\mathcal{D}} + (\mathcal{A}\phi^+, \mathcal{C}^{-1}\mathcal{A}\phi^+)_{\mathcal{D}} \geq \tfrac{1}{2}\|\mathcal{A}\phi^+\|^2_{\mathcal{C}^{-1}} - \tfrac{1}{2}\|\phi^-\|^2_{\mathcal{C}}. \end{aligned}$$

(iii) Combining the two estimates, we obtain for $\psi := \phi + \mathcal{C}^{-1}\mathcal{A}\phi^+$ the inequality $b(\phi,\psi) \geq \frac{1}{2}\|\phi\|^2_{\mathbb{W}}$, while $\|\psi\|_{\mathbb{W}} \leq \sqrt{3}\|\phi\|_{\mathbb{W}}$. This yields the first estimate. The second estimate is derived in the same way, but using the testfunction $\psi := \phi - \mathcal{C}^{-1}\mathcal{A}\phi^+$ instead. □

The unique solvability of Problem 1 now is a consequence of the open-mapping theorem. The following statement for variational problems goes back to [21]; see also [6, 7], for the name.

Lemma 3.9 (Babuzka-Aziz lemma)**.** *Let V, W be Hilbert spaces, and $b : V\times W \to \mathbb{C}$, $\ell : W \to \mathbb{C}$ be continuous bilinear and linear forms. Further, let b satisfy the stability conditions*

$$\sup_{\|w\|_W=1} |b(v,w)| \geq \beta\|v\|_V \qquad \text{and} \qquad \sup_{\|v\|_V=1} |b(v,w)| \geq \beta\|w\|_W$$

for some $\beta > 0$ and all $v \in V$ and $w \in W$, respectively. Then there exists exactly one function $v \in V$ such that $b(v,w) = \ell(w)$ for all $w \in W$, and v is bounded by $\|v\|_V \leq \beta^{-1}\|\ell\|_{W'}$.

As usual, W' denotes the dual space here, i.e., the space of bounded linear functionals on W. Since we have already verified the conditions required in the Babuzka-Aziz lemma in Propositions 3.6–3.8, we directly obtain the unique solvability for our variational problem.

Theorem 3.10. *Problem 1 has a unique solution $\phi \in \mathbb{W}$, which satisfies the a-priori bound*

$$\|\phi\|_{\mathbb{W}} \leq 2\sqrt{3}\,\big(\sqrt{2}\|g\|^2_{\partial\mathcal{D}_-} + \underline{\mu}_a^{-1}\|q\|^2_{\mathcal{D}}\big)^{1/2}.$$

Remark 3.11. Using the norm equivalences of Lemma 2.16, one can obtain similar bounds in other norms, e.g. for $\|\phi\|_{\mathbb{V}_0}$ or $\|\phi\|_{\mathbb{V}_1^+\oplus\mathbb{V}_0^-}$. In view of Lemma 3.9, it is also clear that more general data $q \in \mathbb{W}'$and $g \in \mathbb{T}'_-$ are admissible. We leave such generalizations to the reader.

3.3. **A variational formulation based on alternative spaces.** In the derivation of the variational formulation of Section 3, we used the integration-by-parts formula (2.2) to shift the transport operator in the second term of (3.2) to the test function. Alternatively, one could also transform the first term of (3.2) into

$$(\mathcal{A}\phi^+, \psi^-)_{\mathcal{D}} = -(\phi^+, \mathcal{A}\psi^-)_{\mathcal{D}} + (n\cdot s\ \phi^+, \psi^-)_{\partial\mathcal{D}}.$$

Proceeding in the same way as in Section 3.1, we obtain another variational principle, namely

$$\widetilde{b}(\phi,\psi) = \widetilde{\ell}(\psi) \qquad \text{for all } \psi \in \mathbb{V}_1 \tag{3.11}$$

with bilinear and linear forms defined by

$$\begin{aligned}\widetilde{b}(\phi,\psi) &:= (\mathcal{C}\phi,\psi)_{\mathcal{D}} + (\mathcal{A}\phi^-,\psi^+)_{\mathcal{D}} - (\phi^+,\mathcal{A}\psi^-)_{\mathcal{D}} + (|n\cdot s|\ \phi^-,\psi^-)_{\partial\mathcal{D}}\\ \widetilde{\ell}(\psi) &:= (q,\psi)_{\mathcal{D}} - 2(n\cdot s\ g,\psi^-)_{\partial\mathcal{D}_-}\end{aligned}$$

Since only derivatives of the odd components are involved now, the natural space for (3.11) is

$$\widetilde{\mathbb{W}} := \mathbb{V}_0^+ \oplus \mathbb{V}_1^-.$$

This space has again mixed regularity, but the extra spatial regularity is required for the odd components now. Based on these considerations, we arrive at the following alternative weak form of the radiative transfer equation.

Problem 2. *Given $q \in L^2(\mathcal{D})$ and $g \in L^2(\partial\mathcal{D}_-)$, find a function $\phi \in \widetilde{\mathbb{W}}$ which satisfies* (3.11).

Any solution $\phi \in \widetilde{\mathbb{W}}$ of Problem 2 will again be called a *weak solution* of the radiative transfer equation. The results of Section 3 carry over almost verbatim to this alternative formulation, and we therefore state the unique solvability without giving detailed proofs.

Theorem 3.12. *Problem 2 has a unique solution $\phi \in \widetilde{\mathbb{W}}$ which satisfies the a-priori estimate* $\|\phi\|_{\widetilde{\mathbb{W}}} \leq 2\sqrt{3}\big(\sqrt{2}\|g\|^2_{L^2(\partial\mathcal{D}_-)} + \underline{\mu}_a^{-1}\|q\|^2_{L^2(\mathcal{D})}\big)^{1/2}$.

The results of the following two sections are based on the variational setting of Problem 1. All statements however hold almost verbatim also for the alternative setting considered here.

4. Existence of strong solutions

The aim of this section is to demonstrate that any weak solution $\phi \in \mathbb{W}$ of Problem 1 is in fact also a strong solution of the radiative transfer equation. This requires to show that weak solutions are sufficiently regular, i.e., $\phi \in \mathbb{V}_1$, and that they satisfy (2.4)–(2.5).

4.1. **Notation and preliminary results.** For the subsequent analysis, we require some further notation. For convenience of the reader, we present only the statements that are needed later, and provide some proofs and further details in the appendix.

For any point $(r,s) \in \partial\mathcal{D}_\pm$ on the boundary, we define the *time of travel* $\tau(r,s)$ by

$$\tau(r,s) := \sup\{t > 0 : r \mp t's \in \mathcal{R},\ \forall\ 0 \leq t' \leq t\}.$$

By $\widehat{\mathbb{T}}_\pm$, we then denote the completions of $L^2(\partial\mathcal{D}_\pm)$ with respect to the norms induced by

$$(v,w)_{\mathbb{T}_\pm} := (\tau|n\cdot s|\ v,w)_{\partial\mathcal{D}_\pm}$$

Since the boundary $\partial\mathcal{D}$ coincides with the union of $\partial\mathcal{D}_+$ and $\partial\mathcal{D}_-$ up to a set of measure zero, we can define the space $\widehat{\mathbb{T}}$ of measurable functions whose restrictions to $\partial\mathcal{D}_\pm$ are in $\widehat{\mathbb{T}}_\pm$. For our

analysis, we will require the space $\widehat{\mathbb{V}}_1 = \{v \in \mathbb{V}_0 : s\cdot\nabla v \in \mathbb{V}_0\}$ already mentioned in Remark 2.3, which is larger than $\mathbb{V}_1$. Functions in $\widehat{\mathbb{V}}_1$ are regular enough to admit the notion of boundary values, and the traces $\gamma(v)$ of functions $v \in \widehat{\mathbb{V}}_1$ are in $\widehat{\mathbb{T}}$; cf. [20, 11] and Lemma A2. Hence, $\widehat{\mathbb{V}}_1$ can be defined equivalently as

$$\widehat{\mathbb{V}}_1 := \{v \in \mathbb{V}_0 : s\cdot\nabla v \in \mathbb{V}_0 \text{ and } \|\gamma(v)\|_{\widehat{\mathbb{T}}} < \infty\},$$

and $\widehat{\mathbb{V}}_1$ is a Hilbert space when equipped with the scalar product

$$(v,w)_{\widehat{\mathbb{V}}_1} := (v,w)_{\mathcal{D}} + (s\cdot\nabla v, s\cdot\nabla w)_{\mathcal{D}} + (\tau|n\cdot s|\, v, w)_{\partial\mathcal{D}}.$$

Note that, due to the definition of the norms, the trace operator can now be simply bounded by $\|\gamma(v)\|_{\widehat{\mathbb{T}}} \le \|v\|_{\widehat{\mathbb{V}}_1}$ for all $v \in \widehat{\mathbb{V}}_1$. Let us define a further scalar product by

$$(v,w)_{\check{\mathbb{T}}} := (\tau^{-1}|n\cdot s|\, v, w)_{\mathcal{D}}.$$

Since $0 < \tau \le \operatorname{diam}(\mathcal{R})$ a.e. on $\partial\mathcal{D}$, it follows that the associated norm is stronger than that of $\widehat{\mathbb{T}}$, and we can define $\check{\mathbb{T}} := \{v \in \widehat{\mathbb{T}} : \|v\|_{\check{\mathbb{T}}} < \infty\}$, and a further space $\check{\mathbb{V}}_1 := \{v \in \widehat{\mathbb{V}}_1 : \gamma(v) \in \check{\mathbb{T}}\}$ with scalar product

$$(v,w)_{\check{\mathbb{V}}_1} := (v,w)_{\mathcal{D}} + (s\cdot\nabla v, s\cdot\nabla w)_{\mathcal{D}} + (\tau^{-1}\,|n\cdot s| v, w)_{\partial\mathcal{D}}.$$

The space $\check{\mathbb{T}}$ is again just the space of traces of functions in $\check{\mathbb{V}}_1$. The following result clarifies the relation of the spaces $\widehat{\mathbb{T}}$, $\check{\mathbb{T}}$ and $\widehat{\mathbb{V}}_1$, $\check{\mathbb{V}}_1$ to the spaces $\mathbb{T}$ and $\mathbb{V}_1$ considered in the previous sections; for details, we refer to the appendix.

Lemma 4.1. *The inclusions $\check{\mathbb{T}} \subset \mathbb{T} \subset \widehat{\mathbb{T}}$ and $\check{\mathbb{V}}_1 \subset \mathbb{V}_1 \subset \widehat{\mathbb{V}}_1$ are dense and strict.*

The following generalization of Lemma 2.6 now follows almost directly from the definition of the spaces, by Green's theorem, and a density argument.

Lemma 4.2. *The integration-by-parts formula* (2.2) *holds for all functions $v \in \widehat{\mathbb{V}}_1$ and $w \in \check{\mathbb{V}}_1$.*

Lemma 4.2 will allow us to establish regularity of the boundary values of weak solutions, and will be a basic ingredient in the analysis of the following section.

4.2. **Regularity of weak solutions.** Let us return to the weak form (3.5) of the radiative transfer equation, and recall that any weak solution ϕ satisfies

$$\begin{aligned}(\mathcal{C}\phi,\psi)_{\mathcal{D}} - (\phi^-, \mathcal{A}\psi^+)_{\mathcal{D}} + (\mathcal{A}\phi^+, \psi^-)_{\mathcal{D}} + (|n\cdot s|\,\phi^+, \psi^+)_{\partial\mathcal{D}} \\ = (q,\psi)_{\mathcal{D}} - 2(n\cdot s\, g, \psi^+)_{\partial\mathcal{D}_-}\end{aligned} \tag{4.1}$$

for all test functions $\psi \in \mathbb{W}$. To show the existence of strong solutions, we proceed as follows:

Step 1: We show that ϕ is a solution of (2.4) on $\mathcal{D}$, which requires to verify that $\mathcal{A}\phi^- \in \mathbb{V}_0$. Let $\psi_0 \in \mathbb{W}$ be an arbitrary test function with vanishing boundary values $\gamma(\psi_0^+) = 0$. Then, in the sense of distributions, we obtain that

$$\langle \mathcal{A}\phi^-, \psi_0^+\rangle := -(\phi^-, \mathcal{A}\psi_0^+)_{\mathcal{D}} = (-\mathcal{C}\phi^+ + q^+, \psi_0^+)_{\mathcal{D}},$$

where we have used (4.1) for the second equality, and the parity preserving and reversing properties of the operators. Hence $\mathcal{A}\phi^-$ is a regular distribution, i.e.,

$$\mathcal{A}\phi^- = -\mathcal{C}\phi^+ + q^+ \in \mathbb{V}_0. \tag{4.2}$$

As a consequence, we obtain that $\phi^- \in \widehat{\mathbb{V}}_1$, and thus $\phi \in \widehat{\mathbb{V}}_1$. Using the integration-by-parts formula (2.2) for the second term of (4.1), and utilizing that $\gamma(\psi_0^+) = 0$, we obtain that

$$(\mathcal{A}\phi, \psi_0)_{\mathcal{D}} + (\mathcal{C}\phi, \psi_0)_{\mathcal{D}} = (q, \psi_0)_{\mathcal{D}},$$

for all $\psi_0 \in \mathbb{W}$ with $\gamma(\psi_0) = 0$, and density of $C_0^\infty(\mathcal{D}) \subset \mathbb{V}_0$ implies that $\mathcal{A}\phi + \mathcal{C}\phi = q$ a.e. in $\mathcal{D}$.

Step 2: In order to show that the boundary conditions (2.5) are fulfilled, we now test equation (4.1) with a function $\psi^+ \in \check{\mathbb{V}}_1^+$. Applying Lemma 4.2 for the second term of (4.1), and using equation (4.2) yields

$$\begin{aligned} 2(n\cdot s\; g, \psi^+)_{\partial\mathcal{D}_-} &= (q,\psi^+)_{\mathcal{D}} - (\mathcal{C}\phi^+,\psi^+)_{\mathcal{D}} - (\mathcal{A}\phi^-,\psi^+)_{\mathcal{D}} + (n\cdot s\;\phi^-,\psi^+)_{\partial\mathcal{D}} - (|n\cdot s|\phi^+,\psi^+)_{\partial\mathcal{D}} \\ &= 2(n\cdot s\;\phi^+,\psi^+)_{\partial\mathcal{D}_-} + 2(n\cdot s\;\phi^-,\psi^+)_{\partial\mathcal{D}_-}. \end{aligned}$$

Here, we used that $s \mapsto |n\cdot s|\phi^+\psi^+$ and $s \mapsto n\cdot s\,\phi^-\psi^+$ are even functions, in order to transform the boundary integrals over $\partial\mathcal{D}$ into integrals over $\partial\mathcal{D}_-$, similar as in (3.4). Hence, we obtain that $(n\cdot s\; g,\psi^+)_{\partial\mathcal{D}_-} = (n\cdot s\;\phi,\psi^+)_{\partial\mathcal{D}_-}$ for all $\psi^+ \in \check{\mathbb{V}}_1$, and it follows again by a density argument (see Lemma A6) that $\phi = g$ a.e. on $\partial\mathcal{D}_-$. But since $g \in L^2(\partial\mathcal{D}_-)$, we conclude that $\gamma_-(\phi) \in \mathbb{T}_-$. Using the orthogonal splitting of ϕ into even and odd parts, we also obtain that $\gamma_+(\phi) \in \mathbb{T}_+$, and hence $\phi \in \mathbb{V}_1$. Thus ϕ is a strong solution of the radiative transfer equation (2.4)–(2.5).

Summarizing, we have shown that any weak solution in fact is also a strong solution.

Theorem 4.3. *For any $g \in L^2(\partial\mathcal{D}_-)$ and $q \in L^2(\mathcal{D})$, the radiative transfer equation* (2.4)–(2.5) *has a unique strong solution $\phi \in \mathbb{V}_1$, which coincides with the (weak) solution of Problem 1.*

Proof. The above considerations and Lemma 3.1 show that any weak solution also is a strong solution, and vice versa. The result then follows from Theorem 3.10. □

Remark 4.4. For regular data $q \in L^2(\mathcal{D})$ and $g \in L^2(\partial\mathcal{D}_-)$, the weak and strong forms of the radiative transfer equation are equivalent. As mentioned in Remark 3.11, more general data $q \in \mathbb{W}'$ are allowed in Problem 1 (or $q \in \widetilde{\mathbb{W}}'$ in Problem 2), in which case equivalence does no longer hold.

5. Alternative formulations

In this section, we discuss some alternative weak formulations for the radiative transfer equation, and establish connections between them, and to other methods that have been investigated in literature. Our arguments are based on the variational setting of Problem 1, but corresponding results again hold for the alternative setting discussed in Section 3.3.

5.1. **An operator formulation.** Any variational problem with continuous bilinear form is equivalent to a linear operator equation with bounded linear operator. The operator $\mathcal{B} : \mathbb{W} \to \mathbb{W}'$ associated with the bilinear form b of Problem 1 is given by

$$\begin{aligned} \langle \mathcal{B}v, w\rangle_{\mathbb{W}'\times\mathbb{W}} &:= b(v,w) \\ &= (\mathcal{A}v^+, w^-)_{\mathcal{D}} - (v^-, \mathcal{A}w^+)_{\mathcal{D}} + (\mathcal{C}v, w)_{\mathcal{D}} + (|n\cdot s|\; v^+, w^+)_{\partial\mathcal{D}_-}. \end{aligned}$$

We then consider the following operator formulation of the radiative transfer equation:

Problem 3. *Given $g \in L^2(\partial\mathcal{D}_-)$ and $q \in L^2(\mathcal{D})$, find $\phi \in \mathbb{W}$ such that*

$$\mathcal{B}\phi = \ell \qquad \text{in } \mathbb{W}'. \tag{5.1}$$

The next statement follows almost directly from the results of the previous section.

Lemma 5.1. *The operator $\mathcal{B} : \mathbb{W} \to \mathbb{W}'$ associated with the bilinear form b is continuous and boundedly invertible, i.e., $\|\mathcal{B}\phi\|_{\mathbb{W}'} \le 2\|\phi\|_{\mathbb{W}}$ and $\|\mathcal{B}^{-1}q\|_{\mathbb{W}} \le 2\sqrt{3}\|q\|_{\mathbb{W}'}$ for all $\phi \in \mathbb{W}$ and $f \in \mathbb{W}'$. Moreover, the Problems 1 and 3 are equivalent, and therefore* (5.1) *has a unique solution $\phi \in \mathbb{W}$.*

Proof. By $\langle \mathcal{B}v, w\rangle_{\mathbb{W}'\times\mathbb{W}} = b(v,w)$, the boundedness of the operator follows from Proposition 3.7. The invertibility is a direct consequence of the inf-sup conditions stated in Proposition 3.8, which imply the injectivity and surjectivity of the operator $\mathcal{B}$, respectively. In particular, the first inf-sup condition implies $\beta\|\phi\|_{\mathbb{W}} \le \|\mathcal{B}\phi\|_{W'}$, which provides the bound on the inverse. The equivalence follows by testing the operator equation with $\psi \in \mathbb{W}$ and the definition of the operator, and the unique solvability is inherited from the variational problem. □

Remark 5.2. The operator equation (5.1) is a weak form of the radiative transfer equation, i.e., (2.4)–(2.5) is understood in a distributional sense. Note that, in general, a function $\phi \in \mathbb{W}$ does not have enough regularity to be a candidate for a strong solution. As we have shown in Section 4, any weak solution of Problem 1 or Problem 3, however, has the required extra regularity.

5.2. **A mixed variational problem.** Due to the orthogonality of the splitting $\mathbb{W} = \mathbb{V}_1^+ \oplus \mathbb{V}_0^-$, the energy space $\mathbb{W}$ can be identified with the product space $\mathbb{V}_1^+ \times \mathbb{V}_0^-$. Recalling that $\mathbb{V}_1^+ = \mathbb{W}^+$ and $\mathbb{V}_0^- = \mathbb{W}^-$, we arrive at the following mixed variational formulation.

Problem 4. *Find* $(\phi^+, \phi^-) \in \mathbb{W}^+ \times \mathbb{W}^-$ *such that for all* $\psi^+ \in \mathbb{W}^+$ *and* $\psi^- \in \mathbb{W}^-$ *there holds*

$$(\mathcal{C}\phi^+, \psi^+)_{\mathcal{D}} + (|n\cdot s|\, \phi^+, \psi^+)_{\partial\mathcal{D}} - (\phi^-, \mathcal{A}\psi^+)_{\mathcal{D}} = (q^+, \psi^+)_{\mathcal{D}} + 2(|n\cdot s|\, g, \psi^+)_{\partial\mathcal{D}_-}, \tag{5.2}$$

$$(\mathcal{A}\phi^+, \psi^-)_{\mathcal{D}} + (\mathcal{C}\phi^-, \psi^-)_{\mathcal{D}} = (q^-, \psi^-)_{\mathcal{D}}. \tag{5.3}$$

Remark 5.3. Multiplying the second equation by minus one allows to transform the mixed problem into symmetric form. This was already used implicitly in the proof of Proposition 3.8.

As a direct consequence of the properties of the operators, and the analysis of the previous section, we obtain the following result.

Lemma 5.4. *Problem 1 and Problem 4 are equivalent. In particular, for any* $g \in L^2(\partial\mathcal{D}_-)$ *and* $q \in L^2(\mathcal{D})$*, Problem 4 has a unique solution* $(\phi^+, \phi^-) \in \mathbb{W}^+ \times \mathbb{W}^-$.

Proof. The equivalence follows by identifying $(\psi^+, \psi^-) \in \mathbb{W}^+ \times \mathbb{W}^-$ with $\psi = \psi^+ + \psi^- \in \mathbb{W}$, using the parity preserving and reversing properties of the operators, respectively, and adding the two equations. The unique solvability then follows from Theorem 3.10. □

5.3. **Even-parity formulation.** We show now, that the mixed variational problem (5.2)–(5.3) can be reduced to a single equation by explicitly eliminating the odd parity component ϕ^-. We start with rewriting Problem 4 as equivalent operator equation: Let us define an operator

$$\mathcal{E} : \mathbb{W}^+ \to (\mathbb{W}^+)', \qquad \langle \mathcal{E}v, w\rangle := (|n\cdot s|\, v, w)_{\partial\mathcal{D}} \qquad \text{for } v, w \in \mathbb{W}^+,$$

which is used in order to reformulate the boundary term on the left hand side of equation 5.2. Similarly, we define a linear functional

$$e : \mathbb{W}^+ \to \mathbb{R}, \qquad e(v) := 2(|n\cdot s|\, g, v)_{\partial\mathcal{D}_-} \qquad \text{for } v \in \mathbb{W}^+.$$

to represent the boundary integral on the right. Problem 4 can then be written equivalently as

$$\mathcal{C}\phi^+ + \mathcal{E}\phi^+ - \mathcal{A}^*\phi^- = q^+ + e \qquad \text{in } (\mathbb{W}^+)', \tag{5.4}$$

$$\mathcal{A}\phi^+ + \mathcal{C}\phi^- = q^- \qquad \text{in } (\mathbb{W}^-)', \tag{5.5}$$

where the adjoint operator $\mathcal{A}^* : \mathbb{W}^- \to \mathbb{V}_0^+$ is defined as usual by duality, i.e,

$$\langle \mathcal{A}^*\phi^-, \psi^+\rangle := (\phi^-, \mathcal{A}\psi^+)_{\mathcal{D}}.$$

Since the operator $\mathcal{C} : \mathbb{V}_0 \to \mathbb{V}_0$ is invertible, we can express ϕ^- using (5.5) as

$$\phi^- = \mathcal{C}^{-1}(q^- - \mathcal{A}\phi^+), \tag{5.6}$$

which makes sense in $\mathbb{V}_0$. Inserting this expression for ϕ^- into the first equation (5.4), and rearranging the terms, yields the following operator equation

$$\mathcal{A}^*\mathcal{C}^{-1}\mathcal{A}\phi^+ + \mathcal{C}\phi^+ + \mathcal{E}\phi^+ = \mathcal{A}^*\mathcal{C}^{-1}q^- + q^+ + e \qquad \text{in } (\mathbb{W}^+)'. \tag{5.7}$$

By testing with an arbitrary function $\psi^+ \in \mathbb{W}^+$, we arrive at an equivalent variational principle

$$b_{ep}(\phi^+, \psi^+) = \ell_{ep}(\psi^+) \qquad \text{for all } \psi^+ \in \mathbb{W}^+, \tag{5.8}$$

with bilinear and linear forms defined by

$$b_{ep}(\phi^+, \psi^+) := (\mathcal{C}^{-1}\mathcal{A}\phi^+, \mathcal{A}\psi^+)_{\mathcal{D}} + (\mathcal{C}\phi^+, \psi^+)_{\mathcal{D}} + (|n\cdot s|\, \phi^+, \psi^+)_{\partial\mathcal{D}}$$

$$\ell_{ep}(\psi^+) := (\mathcal{C}^{-1}q^-, \mathcal{A}\psi^+)_{\mathcal{D}} + (q^+, \psi^+)_{\mathcal{D}} - 2(n\cdot s\, g, \psi^+)_{\partial\mathcal{D}_-}.$$

We thus obtain the following reduced variational problem for the even part of the solution.

Problem 5. *Given $q \in L^2(\mathcal{D})$ and $g \in L^2(\partial\mathcal{D}_-)$, find $\psi^+ \in \mathbb{W}^+$ such that* (5.8) *holds.*

Remark 5.5. The form (5.7) or (5.8) is usually referred to as the *even parity* or *second order* form of the radiative transfer equation [18].

The following statements follow almost directly from the results of the previous sections.

Lemma 5.6. *The linear form $\ell_{ep} : \mathbb{W}^+ \to \mathbb{R}$ is bounded, i.e., $|\ell_{ep}(\psi^+)| \le C_l \|\psi^+\|_{\mathbb{W}}$, with C_l as in Proposition 3.6, and $b_{ep} : \mathbb{W}^+ \times \mathbb{W}^+ \to \mathbb{R}$ is continuous and coercive with constants one.*

Proof. The bilinear form $b_{ep} : \mathbb{W}^+ \times \mathbb{W}^+ \to \mathbb{R}$ is exactly the scalar product associated with $\mathbb{W}^+$, which implies coercivity and boundedness. The bound for ℓ_{ep} follows from Proposition 3.6. □

Existence of a unique solution to Problem 5 now follows from the Lax-Milgram theorem.

Theorem 5.7. *Problem 5 has a unique solution $\phi^+ \in \mathbb{W}^+$ with $\|\phi^+\|_{\mathbb{W}} \le (\sqrt{2}\|g\|^2_{\partial\mathcal{D}_-} + \underline{\mu}_a^{-1}\|q\|^2_{\mathcal{D}})^{1/2}$.*

Defining ϕ^- as in (5.6), one easily sees that the pair (ϕ^+, ϕ^-) solves the the mixed operator equation (5.4)–(5.5) and hence Problem 4. The following result then follows from Lemma 5.4.

Theorem 5.8. *The even parity Problem 5 and the variational Problem 1 are equivalent.*

Remark 5.9. A combination of Theorems 5.8 and 5.7 allows to improve the a-priori bound for the solution of Problem 1. Using the definition of ϕ^-, we obtain $\|\phi^-\|^2_{\mathcal{C}} = \|q^-\|^2_{\mathcal{C}^{-1}} + \|\mathcal{A}\phi^+\|^2_{\mathcal{C}^{-1}} - (q^-, \mathcal{C}^{-1}\mathcal{A}\phi^+)_{\mathcal{D}} \le \frac{3}{2}\underline{\mu}_a^{-1}\|q\|^2_{\mathcal{D}} + \frac{3}{2}\|\mathcal{A}\phi^+\|^2_{\mathcal{C}^{-1}}$, and using the a-priori bound of Theorem 5.7 yields the sharper estimate $\|\phi\|_{\mathbb{W}} \le 2\big(\sqrt{2}\|g\|^2_{\partial\mathcal{D}_-} + \underline{\mu}_a^{-1}\|q\|^2_{\mathcal{D}}\big)^{1/2}$.

Remark 5.10. The even parity form of the radiative transfer equation has been used and investigated intensively [18, 1]. As a direct consequence of the coercivity of the bilinear form b_{ep}, it can be shown to be the Euler-Lagrange equation of a certain energy functional [18]. Note that, as Theorem 5.8 states, there is virtually no difference between the mixed problem and the even parity formulation from an analytical point of view.

Remark 5.11. A numerical treatment of the even parity formulation is usually more convenient than the solution of the mixed problem, since it involves less unknowns and additionally leads to self-adjoint systems. This also explains the popularity of the method to some extent. Note that some relevant quantities, like the total outflux of particles defined by

$$(J\cdot n)(r) := \int_{n\cdot s>0} \phi(r,s) n\cdot s \,\mathrm{d}s = \int_{\mathcal{S}} \phi^+ |n\cdot s| \,\mathrm{d}s + \int_{n\cdot s<0} g(r,s) n\cdot s \,\mathrm{d}s,$$

only depend on the even part ϕ^+ of the solution, and thus can be computed without explicit knowledge of the odd component ϕ^-. For curiosity, let us mention that $J\cdot n$ can be computed as well from knowledge of ϕ^- alone, if the alternative approach of Section 3.3 is used.

5.4. **Least-squares formulations.** Let us return to the operator equation of Section 5.1. In the usual way, we define the adjoint operator $\mathcal{B}^* : \mathbb{W} \to \mathbb{W}'$ by duality, i.e.,

$$\langle v, \mathcal{B}^* w\rangle_{\mathbb{W}\times\mathbb{W}'} := b(v,w) = \langle \mathcal{B}v, w\rangle_{\mathbb{W}'\times\mathbb{W}}, \qquad v, w \in \mathbb{W}.$$

Multiplying (5.1) by $\mathcal{B}^*$ from the left yields the *normal equations*

$$\mathcal{B}^*\mathcal{B}v = \mathcal{B}^*\ell \qquad \text{in } \mathbb{W}', \tag{5.9}$$

which are the optimality conditions for the least-squares problem

$$\text{Find } v \in \mathbb{W}: \quad J(v) = \min_{w\in\mathbb{W}} J(w) \qquad \text{with} \quad J(w) = \|\mathcal{B}w - \ell\|^2_{\mathbb{W}'}. \tag{5.10}$$

The following result can be deduced from the properties of the operator $\mathcal{B}$ by standard arguments.

Lemma 5.12. *The least-squares problem* (5.10) *has a unique solution, which coincides with the unique solution of the normal equations* (5.9)*. Both problems are equivalent to Problem 1.*

Proof. The operator $\mathcal{B}^*\mathcal{B}$ is coercive, i.e., $\langle \mathcal{B}^*\mathcal{B}v, v\rangle_{\mathbb{W}\times\mathbb{W}} = \|\mathcal{B}v\|^2_{\mathbb{W}'} \geq \beta^2\|v\|^2_{\mathbb{W}}$, which follows from Proposition 3.8, and the equivalence of Problem 1 with the operator equation of Lemma 5.1. Moreover, (5.9) are the necessary first order optimality conditions for (5.10), which shows uniqueness of a minimizer, and due to the coercivity of $\mathcal{B}^*\mathcal{B}$, the functional J is coercive, which grants the existence. Since $\mathcal{B}v = \ell$ has a solution, we further have $J(v) = \|\mathcal{B}v - \ell\|^2_{\mathbb{W}'} = 0$, which together with uniqueness shows equivalence with Problem 1. □

Remark 5.13. In [19], the following alternative least-squares formulation, based on the strong form (2.4)–(2.5) of the radiative transfer equation, has been studied. In our notation, the problem reads

$$J(v) = \min_{w\in\mathbb{V}_1^g} J(w) \qquad \text{with} \qquad J(w) := \|\mathcal{A}w + \mathcal{C}w - q\|^2_{\mathbb{V}_0}. \tag{5.11}$$

The set over which is minimized is given by $\mathbb{V}_1^g := \{v \in \mathbb{V}_1 : \gamma_-(v) = g\}$; $g \equiv 0$ was used in [19]. This formulation requires the full regularity $v \in \mathbb{V}_1$ of both, even and odd, components of the test functions, i.e., functions in the set $\mathbb{V}_1^g$ have to be more regular than those required in the least-squares problem (5.10). Also note that the boundary values are now incorporated into the definition of the set $\mathbb{V}_1^g$, and that the norm in which the residual is measured is stronger than that of our approach. The existence of a unique minimizer of (5.11) is proven in [19]. Due to Theorem 4.3, this also follows as a by-product of our results stated in Section 3 and 4.

One motivation of [19, 20] for studying the least-squares problem (5.11) was, that due to the coercivity of the least-squares functional, Galerkin methods can be applied for the numerical solution of the radiative transfer equation. As we will demonstrate in the next section, this is also the case for the variational setting considered in this paper.

6. Galerkin approximation

Inf-sup stable variational problems like Problem 1 or 4 can be approximated systematically by Galerkin methods. Let $\mathbb{W}_h \subset \mathbb{W}$ be a closed (e.g. finite dimensional) subspace of $\mathbb{W}$. We then consider the following Galerkin approximation of Problem 1:

Problem 6. *Find $\phi_h \in \mathbb{W}_h$ such that $b(\phi_h, \psi_h) = \ell(\psi_h)$ holds for all $\psi_h \in \mathbb{W}_h$.*

For establishing the unique solvability of Problem 6, one has to verify the conditions of the Babuzka-Aziz lemma for the space $\mathbb{W}_h$. Note that the conditions of Lemma 3.9 are not only sufficient, but also necessary for the existence of a unique solution for all admissible data [6, 7].

Since $\mathbb{W}_h \subset \mathbb{W}$, the boundedness of the bilinear and linear forms follows directly from Propositions 3.6 and 3.7. The corresponding inf-sup conditions however depend on the careful construction of the space $\mathbb{W}_h$, and do not follow from Proposition 3.8. If the *discrete* inf-sup conditions

$$\sup_{\psi_h\in\mathbb{W}_h} \frac{b(\phi_h,\psi_h)}{\|\psi_h\|_{\mathbb{W}}} \geq \beta_h\|\phi_h\|_{\mathbb{W}} \qquad \text{and} \qquad \sup_{\psi_h\in\mathbb{W}_h} \frac{b(\psi_h,\phi_h)}{\|\psi_h\|_{\mathbb{W}}} \geq \beta_h\|\phi_h\|_{\mathbb{W}}, \tag{6.1}$$

hold with a constant $\beta_h > 0$ for all $\phi_h \in \mathbb{W}_h$, then the unique solvability of Problem 6 is granted.

Theorem 6.1. *Assume that* (6.1) *holds for all ϕ_h, $\psi_h \in \mathbb{W}_h$ with some $\beta_h > 0$. Then Problem 6 has a unique solution $\phi_h \in \mathbb{W}_h$, which satisfies $\|\phi_h\|_{\mathbb{W}} \leq \beta_h^{-1}(\sqrt{2}\|g\|^2_{\partial\mathcal{D}_-} + \underline{\mu}_a^{-1}\|q\|^2_{\mathcal{D}})^{1/2}$. Moreover, if $\phi \in \mathbb{W}$ denotes the solution of Problem 1, then*

$$\|\phi - \phi_h\|_{\mathbb{W}} \leq 2\beta_h^{-1} \inf_{v_h\in\mathbb{W}_h} \|\phi - v_h\|_{\mathbb{W}}, \tag{6.2}$$

i.e., the error of the Galerkin approximation is bounded by the best approximation error.

Proof. Solvability follows by application of the Babuzka-Aziz lemma. The quasi best-approximation result is due to [6] with improvement of the constant as in [25]. □

Let us discuss the construction of stable approximation spaces $\mathbb{W}_h$: In the proof of Proposition 3.8, we explicitly used that $\mathcal{A}w^+ \in \mathbb{W}^-$ for all $w^+ \in \mathbb{W}^+$ for the construction of a suitable test function. If this condition is satisfied also on the discrete level, then the discrete stability conditions hold with the same stability constant $\beta_h = \beta$ as on the continuous level.

Proposition 6.2. *Let $\mathbb{W}_h$ be such that $\mathcal{A}w_h^+ \in \mathbb{W}_h^-$ for all $w_h^+ \in \mathbb{W}_h^+$. Then the discrete inf-sup conditions* (6.1) *hold with stability constant $\beta_h = (2\sqrt{3})^{-1}$.*

Proof. The proof of Proposition 3.8 applies almost verbatim. □

Let us further investigate the design of stable discretizations: Due to the tensor product structure of the underlying domain $\mathcal{D} = \mathcal{R} \times \mathcal{S}$, it seems natural (but is not necessary) to consider also tensor product approximations. In the following, we consider a spherical harmonics expansion [12] for discretization of the angular domain, while for the spatial variable, we utilize a finite element approach. We only discuss this particular case in detail here, but other discretization schemes can be treated with similar arguments. For details on various approximations and some numerical results, we refer to [13].

6.1. **P_N-expansion.** For ease of presentation, we confine ourselves to the two dimensional case in the following. The *spherical harmonics* $\{H_n\}_{n\in\mathbb{Z}}$ are then defined by

$$H_n(s) = (2\pi)^{-1/2} e^{in\alpha}, \qquad \text{with} \qquad s = (\cos\alpha, \sin\alpha)^\top,$$

and they form an orthonormal system in $L^2(\mathcal{D})$. Thus, any function $\phi \in L^2(\mathcal{D})$ can be expanded into a Fourier series

$$\phi(r,s) = \sum \phi_n(r) H_n(s) \tag{6.3}$$

with $\phi_n \in L^2(\mathcal{R})$ for $n \in \mathbb{Z}$. If not stated otherwise, the summation will always be carried out over $\mathbb{Z}$. The even and odd components of ϕ are simply given by

$$\phi^+(r,s) = \sum \phi_{2n}(r) H_{2n}(s) \qquad \text{and} \qquad \phi^-(r,s) = \sum \phi_{2n+1}(r) H_{2n+1}(s).$$

Remark 6.3. The Fourier coefficients of a function $\phi \in \mathbb{W}$ with mixed regularity have the following properties: $\phi_{2n+1} \in L^2(\mathcal{R})$ and $\phi_{2n} \in \{v \in L^2(\mathcal{R}) : s\cdot\nabla v \in L^2(\mathcal{R})$ a.e. $s \in \mathcal{S}$ and $v|_{\partial\mathcal{R}} \in L^2(\partial\mathcal{R})\} \supset H^1(\mathcal{R})$. In particular, the even coefficients share the higher spatial regularity of the even part $\phi^+ \in \mathbb{V}_1^+$.

The spherical harmonics expansion allows to express the action of the operators involved in the radiative transfer equation (2.4) in a convenient way: Since $\theta(s\cdot s')$ only depends on the product $s\cdot s'$, or equivalently on $\cos(\alpha-\alpha')$, the scattering kernel can be expanded as

$$\theta(r, s\cdot s') = \sum \theta_n(r) H_{-n}(s') H_n(s) \quad \text{with} \quad \theta_n(r) = \int_0^{2\pi} \theta(r, \cos\alpha) \cos(n\alpha)\, d\alpha. \tag{6.4}$$

Moreover, since θ is real valued, we have $\theta_n = \theta_{-n}$, and from (6.4) and the condition (S1)–(S2) on the scattering kernel, we readily obtain that $|\theta_n(r)| \le 1$.

Remark 6.4. For Henyey-Greenstein scattering [14] with anisotropy factor g one can show by direct calculation that $\theta_n = g^n$. If $|g| \le 1$, then the assumptions (S1)–(S2) on the scattering kernel are satisfied, and for $0 \le g \le 1$, the scattering operator is positive semi-definite; cf. Remark 2.17.

The expansion of the scattering kernel allows to express the scattering and removal operators as

$$(\Theta\phi)(r,s) = \sum \theta_n(r)\phi_n(r) H_n(s) \qquad \text{and} \qquad (\mathcal{C}\phi)(r,s) = \sum c_n(r)\phi_n(r) H_n(s), \tag{6.5}$$

with $c_n(r) = \mu_a(r) + \mu_s(r)(1-\theta_n(r))$. Due to the assumptions (C1)–(C2) on the coefficients and the bound $|\theta_n(r)| \le 1$ on the coefficients of the scattering kernel, we obtain that $c_n(r) \ge \underline{\mu}_a > 0$, which again shows that $\mathcal{C}$ is boundedly invertible. Similarly, $|\theta_n(r)| \le 1$ implies the bound $\|\Theta v\|_{\mathbb{V}_0} \le \|v\|_{\mathbb{V}_0}$ on the scattering kernel.

Using the Euler formulas to express the angular variable s in terms of the spherical harmonics, we obtain the following representation for the transport operator:

$$(\mathcal{A}\phi)(r,s) = \sum \frac{1}{2} \begin{pmatrix} H_{n-1}(s) + H_{n+1}(s) \\ iH_{n-1}(s) - iH_{n+1}(s) \end{pmatrix} \cdot \nabla\phi_n(r). \tag{6.6}$$

Remark 6.5. The application of the transport operator alters the order in the expansion by ± 1. For instance, if $\phi \in \operatorname{span}\{H_n\}$, i.e., $\phi(r,s) = \phi_n(r)H_n(s)$, then $\mathcal{A}\phi \in \operatorname{span}\{H_{n-1}, H_{n+1}\}$. We will make explicit use of this "local" action of the transport operator in the following.

6.2. **Mixed P_N-approximations.** A truncation of the spherical harmonics expansion yields a natural discretization for the angular variable. Let us define

$$\mathbb{V}_{0,N} := \Big\{ v(r,s) = \sum_{n=-N}^{N} \phi_n(r) H_n(s) : \phi_n \in L^2(\mathcal{R}) \Big\}.$$

As approximation space for Problem 6, we then consider the space $\mathbb{W}_N := \mathbb{W} \cap \mathbb{V}_{0,N}$ with norm inherited from $\mathbb{W}$. The following result establishes an important property of the P_N-approximation.

Lemma 6.6. *Let N be odd. Then for every $v \in \mathbb{W}_N^+$ we have $\mathcal{A}v \in \mathbb{W}_N^-$.*

Proof. Set $K = (N-1)/2$. Then the even and odd parts of a function $v \in \mathbb{W}_N$ are given by

$$v^+(r,s) = \sum_{k=-K}^{K} v_{2k}(r) H_{2k}(s) \qquad \text{and} \qquad v^-(r,s) = \sum_{k=-K-1}^{K} v_{2k+1}(r) H_{2k+1}(s).$$

The result then follows by (6.6), and noting that the v_{2k} have the required spatial regularity. □

As a consequence of Lemma 6.6 and Proposition 6.2, we obtain that the discrete inf-sup conditions (6.1) hold for the P_N-approximation with N odd with the same constant $\beta_h = \beta$ as on the continuous level.

Theorem 6.7. *Assume that N is odd, and set $\mathbb{W}_h := \mathbb{W}_N$. Then $b : \mathbb{W}_h \times \mathbb{W}_h \to \mathbb{C}$ is inf-sup stable with constant $\beta_h = (2\sqrt{3})^{-1}$. Moreover, the semi-discrete variational Problem 6 has a unique solution $\phi_h \in \mathbb{W}_h$, which satisfies the a-priori bound $\|\phi_h\|_{\mathbb{W}} \le 2\sqrt{3}(\sqrt{2}\|g\|^2_{\partial\mathcal{D}_-} + \underline{\mu}_a^{-1}\|q\|^2_{\mathcal{D}})^{1/2}$, and the quasi best-approximation estimate* (6.2) *holds.*

Remark 6.8. The fact that *odd* order P_N approximations are "more stable", is frequently reported in literature. Our analysis allows to shed some light onto such statements: Note that an even order approximation of $\mathbb{W}$ would not satisfy the conditions of Proposition 6.2, and therefore the inf-sup stability of the discrete problem could not be granted so easily. The picture changes, however, if we consider the alternative variational setting of Section 3.3. For the space $\widetilde{\mathbb{W}}$, the *even* order P_N approximations are the stable ones, while stability of P_N approximations with N odd is not ensured by Proposition 6.2. We conclude that, in view of Theorem 6.1, even and odd order approximations both deliver the best-approximation error, if only the correct variational setting is used.

6.3. **Full discretization.** Let us now turn to the spatial discretization of the P_N approximation, which is obtained by choosing finite dimensional subspaces for the coefficient functions $\phi_n(r)$ in the expansions. Based on our analysis, it is natural to utilize two different spaces $\mathbb{X}_1^h$ and $\mathbb{X}_0^h$ for the even and odd components ϕ_{2k} and ϕ_{2k+1}, respectively. We assume that the spaces satisfy

$$\mathbb{X}_1^h \subset H^1(\mathcal{R}) \qquad \text{and} \qquad \nabla \mathbb{X}_1^h \subset (\mathbb{X}_0^h)^d. \tag{6.7}$$

These conditions are satisfied easily by appropriate finite element spaces, e.g., by using continuous, piecewise linear Lagrange elements for $\mathbb{X}_1^h$, and piecewise constant discontinuous elements for the space $\mathbb{X}_0^h$. The fully discrete approximation space is then defined as $\mathbb{W}_h := \mathbb{W}_{h,N}^+ \oplus \mathbb{W}_{h,N}^-$, with

$$\mathbb{W}_{h,N}^+ = \Big\{ v(r,s) = \sum_{k=-K}^{K} \phi_{2k}(r) H_{2k}(s) : \phi_{2k} \in \mathbb{X}_1^h \Big\} \qquad \text{and}$$

$$\mathbb{W}_{h,N}^- = \Big\{ v(r,s) = \sum_{k=-K-1}^{K} \phi_{2k+1}(r) H_{2k+1}(s) : \phi_{2k+1} \in \mathbb{X}_0^h \Big\}.$$

Note that by definition of the spaces, the even functions have the required spatial regularity, so we are in the regime of a conforming Galerkin approximation. It then follows from (6.7) that the conclusions of Lemma 6.6 and Theorem 6.7 hold verbatim also for the fully discrete space $\mathbb{W}_h$.

Remark 6.9. The condition $\nabla \mathbb{X}_1^h \subset (\mathbb{X}_0^h)^d$ allows to eliminate the odd parity components explicitly, like in Section 5.3, also on the discrete level. Note that, since the space $\mathbb{X}_0^h$ does not require continuity, this elimination can be done locally (in space). The resulting Schur complement system then is a valid discretization for the even parity formulation of the radiative transfer equation.

Remark 6.10. Discretizations based on a combination of spherical harmonics and finite element methods are frequently used for the numerical solution of the even-parity formulation [23, 4, 5]. Alternative approximations based on discrete ordinates and finite differences are for instance discussed in [15]; see also [16, 3] or [17] for other finite element discretizations. As a third alternative, let us also mention sparse wavelet finite element discretizations investigated in [22], which were used for solving the least-squares problem (5.11) proposed in [19]. A detailed study of various discretizations based on the variational setting discussed in this paper, and numerical results are presented in [13]. Also adaptive approximations of the space $\mathbb{W}$, based on the arguments of this paper, are discussed there.

7. Conclusions

In this paper, we propose a rigorous mixed variational framework for the analysis and numerical approximation of the stationary monochromatic radiative transfer equation. This framework allows to establish the existence and uniqueness of weak solutions, which in turn can be shown to be strong solutions of the radiative transfer equation.

As a by-product of our analysis, we obtain simple conditions that allow to establish stability and quasi-optimal error estimates for a wide class of Galerkin approximations. In particular, we can show that even and odd order P_N approximations, both, yield stable discretizations, if the correct variational setting is used. Moreover, we can give a rigorous derivation of the second order (even parity) form of the radiative transfer equation, which can be shown to be the Schur-complement system of a corresponding mixed formulation of the full radiative transfer equation.

Although we confined ourselves to stationary monochromatic equations, the variational approach proposed in this paper seems to be directly applicable to the transient case, and may be helpful also for the treatment of multigroup transport problems. Extensions in these directions, and a demonstration of the advantages of our approach for the discretization, including numerical validation, is part of ongoing research.

Acknowledgements

The authors would like to thank for support by the Austrian Science Fund (FWF) through grant SFB/F032 and the German Research Foundation (DFG) for support through grant GSC 111.

Appendix

Let the assumptions and notations of Section 2.1 and 4.1 hold.

Lemma A1. *The in- and outflow boundaries $\partial\mathcal{D}_-$ and $\partial\mathcal{D}_+$ are open subsets of $\partial\mathcal{D}$, and $\partial\mathcal{D}_0$ is a closed subset of $\partial\mathcal{D}$ with $(2d-2)$-dimensional measure zero.*

Proof. Due to the regularity of the boundary, the mapping $(r,s) \to n \cdot s$ is continuous, and hence the set $\partial\mathcal{D}_0$ is closed. With the same arguments, $\partial\mathcal{D}_-$ and $\partial\mathcal{D}_+$ are open. Since $\partial\mathcal{R} \in C^1$, it is locally diffeomorphic to a subset of $\mathbb{R}^{d-1}$. Note that in these local coordinates the unit outward normal vector is $(0,\dots,0,-1) \in \mathbb{R}^d$. A standard parametrization of the sphere $\mathcal{S}$ and the product structure of $\partial\mathcal{D}_-$, $\partial\mathcal{D}_+$, $\partial\mathcal{D}_0 \subset \partial\mathcal{R} \times \mathcal{S}$ yield the assertion. □

Lemma A2. *The partial trace operators $\gamma_\pm : \widehat{\mathbb{V}}_1 \to \widehat{\mathbb{T}}_\pm$ are bounded surjections, and*

$$\|\gamma_\pm(v)\|_{\widehat{\mathbb{T}}_\pm} \le C \|v\|_{\widehat{\mathbb{V}}_1}.$$

Proof. The case for the outflow boundary is proven in [20]. The result for the inflow part follows in the same way. □

Remark A3. For the proof of the surjectivity, a "flat" extension $\psi_f \in \mathbb{V}_1$ which is constant along the characteristic lines $r + ts$ is used in [20]. Results concerning the trace operator can also be found in [11], where conditions are given, under which the combined trace operator γ can be shown to be surjective onto a certain subspace of $\widehat{\mathbb{T}}$.

The next statement essentially follows from the fact that $|n\cdot s| \leq 1$ and $0 < \tau \leq \operatorname{diam}(\mathcal{R})$ on $\partial\mathcal{D}_\pm$.

Lemma A4. *The following inclusions are strict and dense*

$$\{v \in C^\infty(\partial\mathcal{D}) : \|v\|_{\check{\mathbb{T}}} < \infty\} \subset \check{\mathbb{T}} \subset \mathbb{T} \subset \widehat{\mathbb{T}}.$$

Proof. In [20], the density $C^\infty(\partial\mathcal{D}_-) \subset \mathbb{T} \subset \widehat{\mathbb{T}}$ is shown. The results carry over verbatim to the outflow boundary, and hence to the whole boundary, since $\partial\mathcal{D}_0$ has measure zero. □

The following density results then are direct consequences of the definition of the spaces.

Corollary A5. *The inclusions $\check{\mathbb{V}}_1 \subset \mathbb{V}_1 \subset \widehat{\mathbb{V}}_1$ are dense and strict.*

Lemma A6. *Let $v \in \widehat{\mathbb{V}}_1$. If $(n\cdot s\, v, w^+)_{\partial\mathcal{D}_-} = 0$ for all $w^+ \in \check{\mathbb{V}}_1^+$, then $v = 0$ on $\partial\mathcal{D}_-$.*

Proof. The proof is based on an standard argument and even extension. Without loss of generality assume v is continuous. Assume that the assertion does not hold: Then there exists a point $(r_0, s_0) \in \partial\mathcal{D}_-$ with a neighborhood $U \subset \overline{\mathcal{D}}$ such that $n\cdot s\, v$ is strictly positive in U. Now, take the Friedrich's mollification w of the characteristic function of a neighborhood of U, such that the support of the mollification has a positive distance to $\partial\mathcal{D}_0$. Then $w^+(r,s) := \frac{1}{2}(w(r,s) + w(r,-s))$ is well-defined, smooth, zero near $\partial\mathcal{D}_0$, and even; hence $w^+ \in \check{\mathbb{V}}_1^+$. By construction, the trace of w^+ equals one on U. Thus $(n\cdot s\, v, w^+)_{\partial\mathcal{D}_-} > 0$, which yields a contradiction. □

References

[1] R. T. Ackroyd. *Finite Element Methods for Particle Transport: Applications to Reactor and Radiation Physics.* Taylor & Francis, Inc., 1997.

[2] M. L. Adams and E. W. Larsen. Fast iterative methods for discrete-ordinates particle transport calculations. *Progress in Nuclear Energy*, 40(1):3–159, 2002.

[3] M. Asadzadeh. Analysis of a fully discrete scheme for neutron transport in two-dimensional geometry. *SIAM J. Numer. Anal.*, 23:543–561, 1986.

[4] E. D. Aydin, C. R. R de Oliveira, and A. J. H. Goddard. A comparison between transport and diffusion calculations using a finite element-spherical harmonics radiation transport method. *Med. Phys.*, 29(9):2013–2023, 2002.

[5] E. D. Aydin, C. R. R de Oliveira, and A. J. H. Goddard. A finite element-spherical harmonics radiation transport model for photon migration in turbid media. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 84:247–260, 2004.

[6] I. Babuška. Error-bounds for finite element method. *Numer. Math.*, 16:322–333, 1971.

[7] I. Babuška and A. K. Aziz. *Survey lectures on the mathematical foundations of the finite element method*, pages 3–359. The Mathematical foundation of the Finite Element method with Applications to Partial Differential Equations. Academic Press, New York, 1972.

[8] K. M. Case and P. F. Zweifel. Existence and uniqueness theorems for the neutron transport equation. *Defense Documentation Center for scientific and technical Information*, 1963.

[9] K. M. Case and P. F. Zweifel. *Linear transport theory.* Addison-Wesley Publishing Co., Reading, Mass.-London-Don Mills, Ont., 1967.

[10] S. Chandrasekhar. *Radiative Transfer.* Dover Publications, Inc., 1960.

[11] R. Dautray and J. L. Lions. *Mathematical Analysis and Numerical Methods for Science and Technology, Evolution Problems II*, volume 6. Springer, Berlin, 1993.

[12] B. Davison. *Neutron Transport Theory.* Monographs on Physics. Oxford University Press, London, 1957.

[13] H. Egger and M. Schlottbom. Numerical methods for radiative transfer based on mixed variational principles. Technical report, AICES, RWTH Aachen, 2011.

[14] L. G. Henyey and J. L. Greenstein. Diffuse radiation in the galaxy. *Astrophys. J.*, 93:70–83, 1941.

[15] A. H. Hielscher, R. E. Alcouffe, and R. L. Barbour. Comparison of finite-difference transport and diffusion calculations for photon migration in homogeneous and heterogeneous tissues. *Phys. Med. Biol.*, 43:1285–1302, 1998.

[16] C. Johnson and J. Pitkäranta. Convergence of a fully discrete scheme for two-dimensional neutron transport. *SIAM J. Numer. Anal.*, 20:951–966, 1983.

[17] G. Kanschat. Solution of radiative transfer problems with finite elements. In G. Kanschat, E. Meinköhn, R. Rannacher, and R. Wehrse, editors, *Numerical Methods in Multidimensional Radiative Transfer*. Springer-Verlag, Berlin Heidelberg, 2009.
[18] E. E. Lewis and W. F. Miller Jr. *Computational Methods of Neutron Transport*. John Wiley & Sons, Inc., New York Chichester Brisbane Toronto Singapore, 1984.
[19] T. A. Manteuffel and K. J. Ressel. Least-squares finite-element solution of the neutron transport equation in diffusive regimes. *SIAM J. Numer. Anal.*, 35(5):806–835, 1998.
[20] T. A. Manteuffel, K. J Ressel, and G. Starke. A boundary functional for the least-squares finite-element solution for neutron transport problems. *SIAM J. Numer. Anal.*, 2:556–586, 2000.
[21] J. Nečas. Sur une méthode pour résoudre les équations dérivées partielles du type elliptique, voisine de la variationnelle. *Ann. Sc. Norm. Sup.*, 16(4):305–326, 1962.
[22] G. Widmer, R. Hiptmair, and C. Schwab. Sparse adaptive finite elements for radiative transfer. *Journal of Computational Physics*, 227:6071–6105, 2008.
[23] S. Wright, S. R. Arridge, and M. Schweiger. A finite element method for the even-parity radiative transfer equation using the P_N approximation. In G. Kanschat, E. Meinköhn, R. Rannacher, and R. Wehrse, editors, *Numerical Methods in Multidimensional Radiative Transfer*. Springer-Verlag, Berlin Heidelberg, 2009.
[24] S. Wright, M. Schweiger, and S. R. Arridge. Reconstruction in optical tomography using P_N approximations. *Meas. Sci. Technol.*, 18:79–86, 2007.
[25] J. Xu and L. Zikatanov. Some observations on Babuška and Brezzi theories. *Numer. Math.*, 94(1):195–202, 2003.

Institute for Mathematics in Industry and Technology, Reichenhainerstrasse 39, TU Chemnitz, D-09126 Chemnitz, Germany
E-mail address: herbert.egger@tu-chemnitz.de
URL: http://www.tu-chemnitz.de/~egger

Aachen Institute for Advanced Study in Computational Engineering Science, Schinkelstrasse 2, RWTH Aachen, D-52062 Aachen, Germany
E-mail address: schlottbom@aices.rwth-aachen.de
URL: http://www.aices.rwth-aachen.de/people/schlottbom