CHEBYSHEV SPECTRAL-S_N METHOD FOR THE NEUTRON TRANSPORT EQUATION

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ABSTRACT. We study convergence of a combined spectral and (S_N) discrete ordinates approximation for a multidimensional, steady state, linear transport problem with isotropic scattering. The procedure is based on expansion of the angular flux in a truncated series of Chebyshev polynomials in spatial variables that results in the transformation of the multidimensional problems into a set of one-dimensional problems. The convergence of this approach is studied in the context of the discrete-ordinates equations based on a special quadrature rule for the scattering integral. The discrete-ordinates and quadrature errors are expanded in truncated series of Chebyshev polynomials of degree $\leq L$, and the convergence is derived assuming $L \leq \sigma_t - 4\pi\sigma_s$ where σ_t and σ_s are total- and scattering cross-sections, respectively.

1. INTRODUCTION

In this note we develop spectral approximations for two and three dimensional, steady state, linear transport equation with isotropic scattering, in bounded domains. The procedure is based on the expansion of the angular flux in a truncated series of Chebyshev polynomials in the spatial variables. We study the convergence of this method in two dimensional case, where we use a special quadrature rule to discretize in the angular variables, approximating the scalar flux. The similarity of the spectral method to the finite element method is evident: the bases functions have a constant norm and the procedure is to represent the approximate solution as a linear combination of finite number of basis functions (truncated series of Chebyshev polynomials) and then use a variational formulation. The main difference is that: the finite element bases functions are locally supported, whereas the chebyshev polynomials are global functions. See also [6] for further details.

In [16] this approach, with no convergence rate analysis, is considered for a truncated series of general orthogonal polynomials. The detailed study in [16] is carried out for the Legendre polynomials, where an index mix caused that a significant drift term is argued to be of lower order and therefore its contribution is not included in the estimates.

We apply this procedure using Chebyshev polynomials with,e.g., the advantage of having constant weighted-L_2 norms, and give a full convergence study including estimates of the contribution from the whole drift term. The final estimation is via an inverse iterative/induction argument, based on an estimate derived from some elementary properties of Chebyshev polynomials in Appendix I. In our knowledge convergence rate analysis, in this setting, is not considered in the literature.

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Related problems, in different settings, are studied in the nuclear engineering literature, see, e.g., references in Vilhena et al in [16]. Barros and Larsen [4] carried out a spectral nodal method for certain discrete-ordinates problems. Chebyshev spectral methods for radiative transfer problems are studied, e.g., by Kim and Ishimaru in [11] and by Kim and Moscoso in [12]. In, e.g., astrophysical aspects, spectral methods are considered for relativistic gravitation and gravitational radiation by Bonazzola el al in [6]. A multi-domain spectral method is studied by Grandclément et al [10], for scalar and vectorial Poisson equations. C++ software library, developed for multi-domain, is available in public domain (GPL), http://www.lorene.obspm.fr. For more detailed study on Chebyshev spectral method and also approximations by the spectral methods we refer the reader to monographs by Boyd [7] and Bernardi and Maday [5].

An outline of this paper is as follows: In Section 2 we derive the truncated spectral equations in 2 dimensions. In Section 3 we prove that a certain weighted-L_2 norm for the error in the discrete-ordinates approximation of the spectral solution is dominated by that of a quadrature approximation. In Section 4 we construct a special quadrature rule and derive convergence rates for the quadrature error. Combining the results of Sections 3 and 4, we conclude the convergence of the discrete-ordinates for the spectral method. Appendix I is devoted to certain properties of the Chebyshev polynomials, that are frequently used in the paper, and also the proof of a crucial estimate used in the approximation of the contribution from the drift term. Finally in Appendix II we derive the spectral equations in a three dimensional setting.

2. The two-dimensional spectral solution

Consider the two-dimensional linear, steady state, transport equation given by

$$\begin{aligned}\mu\frac{\partial}{\partial x}\Psi(\mathbf{x},\mu,\theta)+\sqrt{1-\mu^2}\cos\theta\frac{\partial}{\partial y}\Psi(\mathbf{x},\mu,\theta)+\sigma_t\Psi(\mathbf{x},\mu,\theta)\\ =\int_{-1}^{1}\int_{0}^{2\pi}\sigma_s(\mu',\theta'\to\mu,\theta)\Psi(\mathbf{x},\mu',\theta')d\theta' d\mu'+S(\mathbf{x},\mu,\theta),\end{aligned} \tag{2.1}$$

in the rectangular domain $\Omega=\{\mathbf{x}:=(x,y):\ -1\le x\le 1,\quad -1\le y\le 1\}$ and the directions in $D=\{(\mu,\theta):\ -1\le\mu\le 1,\quad 0\le\theta\le 2\pi\}$. Here $\Psi(\mathbf{x},\mu,\theta)$ is the angular flux, σ_t and σ_s denote the total- and the differential cross sections, respectively, ($\sigma_s(\mu',\theta'\to\mu,\theta)$ describes the scattering from an assumed pre-collision angular coordinates (μ',θ') to a post-collision coordinates (μ,θ)), and S is the source term. See [14] for the details.

Note that, in the case of one-speed neutron transport equation; taking the angular variable in a disc, this problem would corresponds to a three dimensional case with all functions being constant in the azimuthal direction of the z variable. In this way the actual spatial domain may be assumed to be a cylinder with the cross-section Ω and the axial symmetry in z. Then D will correspond to the projection of the points on the unit sphere (the "speed") onto the unit disc (which coincides with D.) See, [1] for the details.

Given the functions $f_1(y,\mu,\theta)$ and $f_2(x,\mu,\theta)$, describing the incident flux, we seek for a solution of (2.1) subject to the following boundary conditions:

For $0 \le \theta \le 2\pi$, let

$$\Psi(x=\pm 1, y, \mu, \theta) = \begin{cases} f_1(y,\mu,\theta), & x=-1, \quad 0<\mu\le 1, \\ 0, & x=1, \quad -1\le \mu < 0. \end{cases} \tag{2.2}$$

For $-1 < \mu < 1$, let

$$\Psi(x, y=\pm 1, \mu, \theta) = \begin{cases} f_2(y,\mu,\theta), & y=-1, \quad 0<\cos\theta\le 1, \\ 0, & y=1, \quad -1\le \cos\theta < 0. \end{cases} \tag{2.3}$$

Expanding the angular flux $\Psi(\mathbf{x},\mu,\theta)$ in terms of the Chebyshev polynomials, in the y variable, leads to

$$\Psi(\mathbf{x},\mu,\theta) = \sum_{i=0}^{I} \Psi_i(x,\mu,\theta) T_i(y). \tag{2.4}$$

Below we determine the first component, i.e., $\Psi_0(x,\mu,\theta)$ explicitly, whereas the other components, $\Psi_i(x,\mu,\theta),\ i=1,\dots I$, will appear as the unknowns in I one dimensional transport equations: We start to determine $\Psi_0(x,\mu,\theta)$, by inserting (2.4) into the boundary conditions (2.3) at $y=\pm 1$, to find that:

$$\Psi_0(x,\mu,\theta) = f_2(x,\mu,\theta) - \sum_{i=1}^{I} (-1)^i \Psi_i(x,\mu,\theta), \qquad 0<\cos\theta\le 1, \tag{2.5}$$

$$\Psi_0(x,\mu,\theta) = -\sum_{i=1}^{I} \Psi_i(x,\mu,\theta), \qquad -1\le\cos\theta<0. \tag{2.6}$$

where $-1\le x\le 1$, $-1<\mu<1$, and we have used the fact that for the Chebyshev polynomials $T_0(x)\equiv 1$, $T_i(1)\equiv 1$ and $T_i(-1)=(-1)^i$. See Appendix I.

If we now insert Ψ from (2.4) into (2.1), multiply the resulting equation by $\frac{T_k(y)}{\sqrt{1-y^2}}$, $k=1,\dots,I$, and integrate over y we find that the components $\Psi_k(x,\mu,\theta)$, $k=1,....,I$, satisfy the following I one-dimensional transport equations:

$$\begin{aligned} &\mu\frac{\partial}{\partial x}\Psi_k(x,\mu,\theta) + \sigma_t \Psi_k(x,\mu,\theta) \\ &\qquad = \int_{-1}^{1}\int_0^{2\pi} \sigma_s(\mu',\theta'\to\mu,\theta)\Psi_k(x,\mu',\theta')d\theta' d\mu' + G_k(x,\mu,\theta). \end{aligned} \tag{2.7}$$

The same procedure with the boundary condition (2.2) at $x=-1$, and (2.4) yields

$$\Psi(-1,y,\mu,\theta) = f_1(y,\mu,\theta) = \sum_{i=0}^{I} \Psi_i(-1,\mu,\theta)T_i(y). \tag{2.8}$$

Now multiply (2.8) by $\frac{T_k(y)}{\sqrt{1-y^2}}$; $k=1,\dots,I$, and integrating over y we find that

$$\Psi_k(-1,\mu,\theta) = \frac{2}{\pi}\int_{-1}^{1} f_1(y;\mu,\theta)\frac{T_k(y)}{\sqrt{1-y^2}}dy. \tag{2.9}$$

Similarly, (note the sign of μ below), the boundary condition at $x=1$ is written as

$$\sum_{i=0}^{I} \Psi_i(1,-\mu,\theta)T_i(y) = 0, \qquad 0<\mu\le 1. \tag{2.10}$$

Multiplying (2.10) by $\frac{T_k(y)}{\sqrt{1-y^2}}$; $k = 1, \dots, I$ and integrating over y, we get

$$\Psi_k(1, -\mu, \theta) = 0, \qquad 0 < \mu \le 1, \quad 0 \le \theta \le 2\pi. \tag{2.11}$$

We can easily check that G_k in (2.7) is written as

$$G_k(x, \mu, \theta) = S_k(x, \mu, \theta) - \sqrt{1-\mu^2}\cos\theta \sum_{i=k+1}^{I} A_i^k \Psi_k(x, \mu, \theta) \tag{2.12}$$

where

$$A_i^k = \frac{2}{\pi} \int_{-1}^{1} \frac{d}{dy}(T_i(y)) \frac{T_k(y)}{\sqrt{1-y^2}}\, dy \tag{2.13}$$

and

$$S_k(x, \mu, \theta) = \frac{2}{\pi} \int_{-1}^{1} S(x, y, \mu, \theta) \frac{T_k(y)}{\sqrt{1-y^2}} dy. \tag{2.14}$$

Note that the solutions to the one dimensional problems given through the equations (2.7)–(2.14) define the components $\Psi_k(x, \mu, \theta)$ for $k = I, \dots, 1$, in this decreasing order to avoid the coupling of the equations. Once this is done, the angular flux is completely determined by (2.4). Here, we have used the convention $\sum_{i=I+1}^{I} \dots = 0$. Hence, the staring $G_I(x, \mu, \theta) \equiv S_I(x, \mu, \theta)$. Note also that although the solution, developed in here, rely on specific boundary conditions the procedure is quite general in the sense that the expression for the first component, $\Psi_0(x, \mu, \theta)$, keeps the information from the boundary conditions in the y variable, while the other components are derived based on the boundary conditions in x.

3. Convergence of the spectral solution

In the sequel we focus on the two dimensional, steady state linear transport process with *isotropic scattering*, i.e., $\sigma_s(\mu', \theta' \to \mu, \theta) \equiv \sigma_s =$ constant. For this problem we show, using a weighted-L_2 norm, convergence of the spectral solution defined for the spatial variables. More specifically we show that: in a certain weighted- L_2 norm, the (truncated) *discrete ordinates* approximation error for the spectral solution is dominated by that of a special *quadrature error*. The study of convergence of this quadrature approximation is the matter of the next section.

Assuming isotropic scattering, the equation (2.1) is written as

$$\begin{aligned} &\mu \frac{\partial}{\partial x} \Psi(\mathbf{x}, \mu, \theta) + \sqrt{1-\mu^2}\cos\theta \frac{\partial}{\partial y} \Psi(\mathbf{x}, \mu, \theta) + \sigma_t \Psi(\mathbf{x}, \mu, \theta) \\ &\qquad = \sigma_s \int_{-1}^{1} \int_{0}^{2\pi} \Psi(\mathbf{x}, \mu', \theta') d\theta' d\mu' + S(\mathbf{x}, \mu, \theta) \end{aligned} \tag{3.1}$$

for $\mathbf{x} \in \Omega := \{(x, y) : \ -1 \le x \le 1,\ -1 \le y \le 1\}$, $\mu \in [-1, 1]$ and $\theta \in [0, 2\pi]$. The study of the problem with the anisotropic scattering is a rather involved task. See, e.g., [3] for an approach involving anisotropic scattering. Consider now the discrete ordinates (S_N) approximation of the equation (3.1): for $m = 1, ..., M$, let

$$\mu_m \frac{\partial}{\partial x} \Psi_m(\mathbf{x}) + \eta_m \frac{\partial}{\partial y} \Psi_m(\mathbf{x}) + \sigma_t \Psi_m(\mathbf{x}) = \sigma_s \sum_{n=1}^{M} \omega_n \Psi_n(\mathbf{x}) + S_m(\mathbf{x}), \tag{3.2}$$

where

$$\eta_m = \sqrt{1-\mu_m^2}\cos\theta_m, \tag{3.3}$$

and $\Psi_m(\mathbf{x}) := \Psi_m(x,y)$ is the angular flux in the directions defined by μ_m and η_m and associated with the quadrature weights ω_m. Finally $S_m(\mathbf{x})$ is the corresponding inhomogeneous source term defined in the discrete direction $(\mu_m, \eta_m) \in [-1,1]^2$. We assume a quadrature mesh $(\mu_m, \eta_m) \neq (0,0)$,

$$\begin{cases} \mu_1 < \mu_2 < .... < \mu_M, \\ \eta_1 < \eta_2 < ... < \eta_M, \end{cases} \tag{3.4}$$

satisfying the following conditions:

$$\omega_m \sim 4\pi/M, \qquad \sum_{m=1}^{M} \omega_m \sim 4\pi, \qquad m = 1, ..., M. \tag{3.5}$$

Further, we assume that the discrete-ordinates equation (3.2) satisfy the same boundary conditions, in the discrete directions, as the continuous one, i.e., (3.1) (as stated is Section 2). We shall prove that, under certain assumptions, the solution of the equation (3.2) would converge to that of the equation (3.1) as $M \to \infty$. To this approach we define the *error in the approximate flux* by

$$\varepsilon_m(\mathbf{x}) = \Psi(\mathbf{x}, \mu_m, \eta_m) - \Psi_m(\mathbf{x}), \qquad m = 1, ..., M, \tag{3.6}$$

and the *truncation error in the quadrature formula* as

$$\tau(\mathbf{x}) = \int_{-1}^{1} \int_{0}^{2\pi} \Psi(\mathbf{x}; \mu', \theta') d\mu' d\theta' - \sum_{n=1}^{M} \omega_n \Psi(\mathbf{x}, \mu_n, \eta_n). \tag{3.7}$$

Subtracting the discrete ordinates equation (3.2) from the continuous equation (3.1) in the discrete directions, we obtain, for each $m = 1, \ldots, M$, an equation relating the discrete ordinates approximation error to the quadrature error, viz,

$$\mu_m \frac{\partial \varepsilon_m(\mathbf{x})}{\partial x} + \eta_m \frac{\partial \varepsilon_m(\mathbf{x})}{\partial y} + \sigma_t \varepsilon_m(\mathbf{x}) = \sigma_s \sum_{n=1}^{M} \omega_n \varepsilon_n(\mathbf{x}) + \sigma_s \tau(\mathbf{x}). \tag{3.8}$$

We expand both the approximation and the quadrature errors in a truncated series of Chebyshev polynomials in y,

$$\varepsilon_m(\mathbf{x}) = \sum_{l=0}^{L} \varepsilon_m^l(x) T_l(y), \tag{3.9}$$

$$\tau(\mathbf{x}) = \sum_{l=0}^{L} \tau^l(x) T_l(y) \tag{3.10}$$

and define the $l-th$ moments of the errors by

$$\|\varepsilon^l\| = \Big(\frac{2-\delta_{l,0}}{\pi} \int_{-1}^{1} \sum_{m=1}^{M} \omega_m (\varepsilon_m^l(x))^2 dx\Big)^{1/2}, \tag{3.11}$$

$$\|\tau^l\| = \Big(\frac{2-\delta_{l,0}}{\pi} \int_{-1}^{1} (\tau^l(x))^2 dx\Big)^{1/2}. \tag{3.12}$$

Remark. Note that (3.9) and (3.10) involve further, truncated, approximations of $\tau(\mathbf{x})$, in (3.7) and the solution $\varepsilon_m(\mathbf{x})$ of (3.6). We keep using the same notation as before the truncations. Also, despite the recent truncation in y, we use equalities in (3.9), (3.10), as well as in the subsequent relations below.

The main result of this paper is as follows:

Theorem 3.1. *Let $L = \mathcal{O}(\sigma)$, where $\sigma = \sigma_{tr} - 4\pi\sigma_s$, then for $l = 0, 1, \ldots, L$,*

$$\|\varepsilon^l\| \longrightarrow 0, \qquad as \quad M \longrightarrow \infty.$$

In the remaining part of this section we show that, for $\omega_m \sim 4\pi/M$, $m = 1, \ldots, M$, the L_2 norm of the truncated spectral error $\|\varepsilon^l\|$, counted in a reverse order on $l = L, L-1, \ldots, 0$, is dominated by that of the quadrature error $\|\tau^l\|$.

The next section is devoted to proof of the following result:

Theorem 3.2. *For $\omega_m \sim 4\pi/M$, $m = 1, , \ldots, M$, if $\Psi \in L_1(\mu, \theta)$, then*

$$\|\tau^l\| \longrightarrow 0, \qquad as \quad M \longrightarrow \infty.$$

To prepare for the proof of the Theorem 3.1, we substitute (3.9) and (3.10) into the equation (3.8) to get

$$\begin{aligned} \mu_m \sum_{l=0}^{L} \frac{d\varepsilon_m^l(x)}{dx} T_l(y) + \eta_m \sum_{l=0}^{L} \varepsilon_m^l(x) \frac{dT_l}{dy}(y) + \sigma_t \sum_{l=0}^{L} \varepsilon_m^l(x) T_l(y) \\ = \sigma_s \sum_{n=1}^{M} \omega_n \sum_{l=0}^{L} \varepsilon_n^l(x) T_l(y) + \sigma_s \sum_{l=0}^{L} \tau^l(x) T_l(y). \end{aligned} \tag{3.13}$$

Multiplying (3.13) by $\frac{T_j(y)}{\sqrt{1-y^2}}$, $j = 0, \ldots, L$ and integrating over y yields

$$\begin{aligned} \frac{\pi}{2-\delta_{j,0}} \mu_m \frac{d\varepsilon_m^j(x)}{dx} + \eta_m \sum_{l=0}^{L} \gamma_j(l) \varepsilon_m^l(x) + \frac{\pi}{2-\delta_{j,0}} \sigma_t \varepsilon_m^j(x) \\ = \frac{\pi}{2-\delta_{j,0}} \sigma_s \sum_{n=1}^{M} \omega_n \varepsilon_n^j(x) + \frac{\pi}{2-\delta_{j,0}} \sigma_s \tau^j(x), \end{aligned} \tag{3.14}$$

where

$$\gamma_j(l) = \int_{-1}^{1} \frac{dT_l}{dy}(y) \cdot \frac{T_j(y)}{\sqrt{1-y^2}} dy. \tag{3.15}$$

Finally, we multiply the equation (3.14) by $\varepsilon_m^j(x)$ and integrate over x to obtain

$$\begin{aligned} \frac{\pi}{2-\delta_{j,0}} \mu_m \int_{-1}^{1} \varepsilon_m^j(x) \frac{d\varepsilon_m^j(x)}{dx} dx + \eta_m \sum_{l=0}^{L} \gamma_j(l) \int_{-1}^{1} \varepsilon_m^j(x) \varepsilon_m^l(x) dx \\ + \frac{\pi}{2-\delta_{j,0}} \sigma_t \int_{-1}^{1} \left[\varepsilon_m^j(x)\right]^2 dx \\ = \frac{\pi}{2-\delta_{j,0}} \sigma_s \sum_{n=1}^{M} \omega_n \int_{-1}^{1} \varepsilon_m^j(x) \varepsilon_n^j(x) dx + \frac{\pi}{2-\delta_{j,0}} \sigma_s \int_{-1}^{1} \varepsilon_m^j(x) \tau^j(x) dx. \end{aligned} \tag{3.16}$$

Now we rewrite the first term in equation (3.16) as

$$\mu_m \int_{-1}^{1} \varepsilon_m^j(x) \frac{d\varepsilon_m^j(x)}{dx} dx = \frac{\mu_m}{2} \left[(\varepsilon_m^j(1))^2 - (\varepsilon_m^j(-1))^2 \right]. \tag{3.17}$$

Note that $\mu_m[(\varepsilon_m^j(1))^2 - (\varepsilon_m^j(-1))^2] > 0$. Indeed, for $\mu_m > 0$, using the boundary condition $\varepsilon_m(-1, y) = 0$ and the identity

$$\varepsilon_m^j(x) = \frac{2 - \delta_{j,0}}{\pi} \int_{-1}^{1} \varepsilon_m(x, y) T_j(y) \frac{1}{\sqrt{1 - y^2}} dy, \tag{3.18}$$

we find that $\varepsilon_m^j(-1) = 0$. The same is valid for $x = 1$, when $\mu_m < 0$. Consequently,

$$\begin{aligned} \frac{2 - \delta_{j,0}}{\pi} \eta_m \sum_{l=0}^{L} \gamma_j(l) \int_{-1}^{1} \varepsilon_m^j(x) \varepsilon_m^l(x) dx + \sigma_t \int_{-1}^{1} \left[\varepsilon_m^j(x)\right]^2 dx \\ \le \sigma_s \sum_{n=1}^{M} \omega_n \int_{-1}^{1} \varepsilon_m^j(x) \varepsilon_n^j(x) dx + \sigma_s \int_{-1}^{1} \varepsilon_m^j(x) \tau^j(x) dx. \end{aligned} \tag{3.19}$$

To proceed we multiply the inequality (3.19) by ω_m and sum over m to obtain

$$\begin{aligned} \sigma_t \int_{-1}^{1} \sum_{m=1}^{M} \omega_m \left(\varepsilon_m^j(x)\right)^2 dx \le \sigma_s \int_{-1}^{1} & \left[\sum_{m=1}^{M} \omega_m \varepsilon_m^j(x)\right]^2 dx \\ + \sigma_s \int_{-1}^{1} & \left[\sum_{m=1}^{M} \omega_m \varepsilon_m^j(x)\right] \tau^j(x) dx \\ - \frac{2 - \delta_{j,0}}{\pi} \sum_{m=1}^{M} \omega_m & \left[\eta_m \sum_{l=0}^{L} \gamma_j(l) \int_{-1}^{1} \varepsilon_m^j(x) \varepsilon_m^l(x) dx\right] \\ := & \, I + II + III. \end{aligned} \tag{3.20}$$

The crucial part is now to estimate the γ-term III using the elementary properties of the Chebyshev polynomials. We start with the simpler terms I and II:

Lemma 3.3. *With $\omega_m \sim 4\pi/M$, $m = 1, \ldots, M$, we have, for $j = 0, \ldots, L$, that*

$$\begin{aligned} |I| &\le 4\pi \sigma_s \frac{\pi}{2 - \delta_{j,0}} \left\|\varepsilon^j\right\|^2 \\ |II| &\le \sqrt{4\pi} \sigma_s \frac{\pi}{2 - \delta_{j,0}} \left\|\varepsilon^j\right\| \left\|\tau^j\right\| \end{aligned} \tag{3.21}$$

Proof. We use the elementary relation

$$(a_1 + a_2 + \ldots + a_M)^2 \le M(a_1^2 + a_2^2 + \ldots + a_M^2),$$

to write

$$\left[\sum_{m=1}^{M} \omega_m \varepsilon_m^j(x)\right]^2 \le M \max_{1 \le m \le M} |\omega_m| \sum_{m=1}^{M} \omega_m \left[\varepsilon_m^j(x)\right]^2. \tag{3.22}$$

Integrating (3.22) over x and using $\omega_m \sim 4\pi/M$ we get

$$\int_{-1}^{1} \left[\sum_{m=1}^{M} \omega_m \varepsilon_m^j(x)\right]^2 dx \le 4\pi \int_{-1}^{1} \sum_{m=1}^{M} \omega_m \left[\varepsilon_m^j(x)\right]^2 dx, \tag{3.23}$$

and hence the first estimate follows recalling (3.11). As for the second estimate, applying the Cauchy-Schwarz inequality, (3.23), (3.11) and (3.12) we get

$$\begin{aligned}
&\int_{-1}^{1}\left[\sum_{m=1}^{M}\omega_m\varepsilon_m^j(x)\right]\tau^j(x)dx\\
&\qquad\leq\left(\int_{-1}^{1}\left[\sum_{m=1}^{M}\omega_m\varepsilon_m^j(x)\right]^2dx\right)^{1/2}\times\left(\int_{-1}^{1}\left|\tau^j(x)\right|^2dx\right)^{1/2}\\
&\qquad\leq\sqrt{4\pi}\left(\int_{-1}^{1}\sum_{m=1}^{M}\omega_m\left[\varepsilon_m^j(x)\right]^2dx\right)^{1/2}\times\sqrt{\frac{\pi}{2-\delta_{j,0}}}\|\tau^j\|\\
&\qquad\leq\sqrt{4\pi}\frac{\pi}{2-\delta_{j,0}}\|\varepsilon^j\|\|\tau^j\|,
\end{aligned}\tag{3.24}$$

which gives the desired estimate for II and the proof is complete. □

Next using the Proposition 5.1 from the Appendix I we estimate the contribution from the γ term III and derive the following key estimate:

Proposition 3.4. *For $k=0,1,2,\dots,L$, we have the recursive estimates*

$$\|\varepsilon^{L-k}\|\leq\sum_{j=0}^{k}\frac{\left(1-(-1)^{j+k}\right)}{\sigma}(L-j)\|\varepsilon^{L-j}\|+\frac{\sqrt{4\pi}\sigma_s}{\sigma}\|\tau^{L-k}\|.\tag{3.25}$$

Hence, in particular the starting estimate, for $k=0$, is:

$$\|\varepsilon^L\|\leq\frac{\sqrt{4\pi}\sigma_s}{\sigma}\|\tau^L\|.\tag{3.26}$$

With these estimates we can now easily prove our main result:

Proof of Theorem 3.1. Proposition 3.4 and Theorem 3.2 give the desired result. □

Proof of Proposition 3.4. By the Proposition 5.1 (see Appendix I) we have that

$$\gamma_j(l)=0,\qquad\text{for}\quad j\geq l,\tag{3.27}$$

whereas for $j<l$,

$$\gamma_j(l)=\begin{cases}0, & \text{for}\quad j+l\quad\text{even}\\ l\pi, & \text{for}\quad j+l\quad\text{odd.}\end{cases}\tag{3.28}$$

Therefor if we start with $j=L$, then $\gamma_j(L)=0$ and hence (3.20) combined with the definition (3.11) and Lemma 3.3 yields

$$\sigma_t\frac{\pi}{2}\left\|\varepsilon^L\right\|^2\leq4\pi\sigma_s\frac{\pi}{2}\left\|\varepsilon^L\right\|^2+\sqrt{4\pi}\sigma_s\frac{\pi}{2}\left\|\varepsilon^L\right\|\left\|\tau^L\right\|.\tag{3.29}$$

Now rearranging the terms and recalling that $\sigma:=\sigma_t-4\pi\sigma_s$ we obtain (3.26).

The proof of (3.25) is a reversed inductive argument as follows:
For $j=L-1$ we have that $\gamma_j(L)=\gamma_{L-1}(L)=L\pi$, whereas $\gamma_{L-1}(l)=0$, for $l<L$. Hence, using (3.27) we get

$$\sum_{l=0}^{L}\gamma_j(l)\varepsilon_m^l(x)=\sum_{l=0}^{L}\gamma_{L-1}(l)\varepsilon_m^l(x)=\gamma_{L-1}(L)\varepsilon_m^L(x)=L\pi\varepsilon_m^L(x).\tag{3.30}$$

Thus using the Cauchy-Schwarz inequality

$$
\begin{aligned}
|III| =&\Big| -\frac{2-\delta_{j,0}}{\pi}\sum_{m=1}^{M}\omega_m\Big(\eta_m\int_{-1}^{1}\sum_{l=0}^{L}\gamma_{L-1}(l)\varepsilon_m^l(x)\varepsilon_m^{L-1}(x)\,dx\Big)\Big| \\
&\le \frac{2}{\pi}L\pi\int_{-1}^{1}\Big|\sum_{m=1}^{M}\eta_m\omega_m\varepsilon_m^L(x)\varepsilon_m^{L-1}(x)\Big|dx \\
&\le 2L(\max_m|\eta_m|)\Big(\int_{-1}^{1}\sum_{m=1}^{M}\omega_m[\varepsilon_m^L(x)]^2\,dx\Big)^{1/2}\times \\
&\qquad\Big(\int_{-1}^{1}\sum_{m=1}^{M}\omega_m[\varepsilon_m^{L-1}(x)]^2\,dx\Big)^{1/2} \\
&\le 2L\sqrt{\frac{\pi}{2}}\left\|\varepsilon^L\right\|\sqrt{\frac{\pi}{2}}\left\|\varepsilon^{L-1}\right\| = L\pi\left\|\varepsilon^L\right\|\left\|\varepsilon^{L-1}\right\|.
\end{aligned}
\tag{3.31}
$$

Inserting in (3.20) and using also (3.11) and Lemma 3.3, with $j = L-1$, we get

$$
\begin{aligned}
\sigma_t\frac{\pi}{2}\left\|\varepsilon^{L-1}\right\|^2 \le 4\pi\sigma_s\frac{\pi}{2}\left\|\varepsilon^{L-1}\right\|^2 &+ \sqrt{4\pi}\sigma_s\frac{\pi}{2}\left\|\varepsilon^{L-1}\right\|\ \left\|\tau^{L-1}\right\| \\
&+ L\pi\left\|\varepsilon^L\right\|\left\|\varepsilon^{L-1}\right\|,
\end{aligned}
\tag{3.32}
$$

or equivalently using the notation $\sigma = \sigma_t - 4\pi\sigma_s$,

$$
\sigma\left\|\varepsilon^{L-1}\right\| \le 2L\left\|\varepsilon^L\right\| + \sqrt{4\pi}\sigma_s\left\|\tau^{L-1}\right\|. \tag{3.33}
$$

The same procedure applied to $j = L-2$ yields $\gamma_j(L) = \gamma_{L-2}(L) = 0$, (note that here $j+L$ is even), $\gamma_{L-2}(L-1) = (L-1)\pi$ and $\gamma_{L-2}(l) = 0$, for $l < L-1$. Thus

$$
\sum_{l=0}^{L}\gamma_{L-2}(l)\varepsilon_m^l(x) = \gamma_{L-2}(L-1)\varepsilon_m^{L-1}(x) = (L-1)\pi\varepsilon_m^{L-1}(x), \tag{3.34}
$$

so that, as in the previous step

$$
\sigma\left\|\varepsilon^{L-2}\right\| \le 2(L-1)\left\|\varepsilon^{L-1}\right\| + \sqrt{4\pi}\sigma_s\left\|\tau^{L-2}\right\|. \tag{3.35}
$$

Similarly since for $j = L-3$; we have $\gamma_{L-3}(L) = L\pi$, $\gamma_{L-3}(L-1) = 0$, $\gamma_{L-3}(L-2) = (L-2)\pi$ and $\gamma_{L-3}(l) = 0$ for $l < L-2$, we get

$$
\begin{aligned}
\sum_{l=0}^{L}\gamma_{L-3}(l)\varepsilon_m^l(x) &= \gamma_{L-3}(L-2)\varepsilon_m^{L-2}(x) + \gamma_{L-3}(L)\varepsilon_m^L(x) \\
&= 2(L-2)\varepsilon_m^{L-2}(x) + 2L\varepsilon_m^L(x),
\end{aligned}
\tag{3.36}
$$

which using the same procedure as before yields

$$
\sigma\left\|\varepsilon^{L-3}\right\| \le 2L\left\|\varepsilon^L\right\| + 2(L-2)\left\|\varepsilon^{L-2}\right\| + \sqrt{4\pi}\sigma_s\left\|\tau^{L-3}\right\|. \tag{3.37}
$$

Now the formula (3.25) is proved by an induction argument. □

4. The quadrature rule and Proof of Theorem 3.2

In this section we construct a special quadrature mesh satisfying the conditions in (3.5) and prove the Theorem 3.2 in this setting. This would provide us the remaining step in the proof of the Theorem 3.1 and complete the convergence analysis. We also derive convergence rates for the quadrature error (3.7) where we identify the angular domain

$$D = \{(\mu, \theta) : -1 \leq \mu \leq 1,\ 0 \leq \theta \leq 2\pi\}, \tag{4.1}$$

by

$$\tilde{D} := \left\{(\mu, \eta) : -1 \leq \mu,\ \eta \leq 1,\ \eta = \sqrt{1-\mu^2}\cos\theta\right\}. \tag{4.2}$$

Then the quadrature (cubature) rule, for the multiple integral in (3.1) can be constructed using (4.2) as in (3.7), see [9]. To derive convergence rates, below we construct an equivalent rule, directly discretizing D given by (4.1), and with a somewhat general features:

$$\int_0^{2\pi}\int_{-1}^{1}\Psi(\mathbf{x};\mu,\theta)d\mu d\theta \sim \sum_{\Delta}\omega_{kj}\Psi(\mathbf{x},\mu_k,\theta_j), \tag{4.3}$$

where $\Delta := \{(\mu_k, \theta_j),\ k = 1, ..., K \text{ and } j = 1, ..., J,\ J \sim K\} \subset D$ is a $M = JK$, discrete set of points in D consisting of the Gauss quadrature points $\mu_k \in [-1, 1]$ associated with the equally spaced $\theta_j = \frac{2\pi j}{J}$, $j = 1, ..., J$, and weights $\omega_{kj} = A_k W_j$ where $W_j = \frac{2\pi}{J}$, $j = 1, ..., J$ and A_k are given below. Thus the error in (4.3) can be split into two decoupled quadrature errors:

$$\begin{aligned}
|e_M(\Psi)| &:= \Big|\int_0^{2\pi}\int_{-1}^{1}\Psi(\mathbf{x};\mu,\theta)d\mu d\theta - \sum_{\Delta}\omega_{kj}\Psi(\mathbf{x},\mu_k,\theta_j)\Big| \\
&\leq \int_0^{2\pi}\Big|\int_{-1}^{1}\Psi(\mathbf{x};\mu,\theta)d\mu - \sum_{k=1}^{K}A_k\Psi(\mathbf{x},\mu_k,\theta)\Big|d\theta \\
&+ \sum_{k=1}^{K}A_k\Big[\Big|\int_0^{2\pi}\Psi(\mathbf{x},\mu_k,\theta)d\theta - \sum_{j=1}^{J}W_j\Psi(\mathbf{x},\mu_k,\theta_j)\Big|\Big] \\
&:= \int_0^{2\pi}|e_K[\Psi(\mathbf{x},\theta)]|\,d\theta + \sum_{k=1}^{K}A_k|e_J[\Psi(\mathbf{x},\mu_k)]|,
\end{aligned} \tag{4.4}$$

with the obvious notations for the two quadrature errors:

$$e_J[\Psi(\mathbf{x},\mu)] := \int_0^{2\pi}\Psi(\mathbf{x},\mu,\theta)d\theta - \sum_{j=1}^{J}W_j\Psi(\mathbf{x},\mu,\theta_j), \tag{4.5}$$

$$e_K[\Psi(\mathbf{x},\theta)] := \int_{-1}^{1}\Psi(\mathbf{x};\mu,\theta)d\mu - \sum_{k=1}^{K}A_k\Psi(\mathbf{x},\mu_k,\theta). \tag{4.6}$$

Below we derive error estimates for the quadrature rules (4.5) and (4.6), with *optimal* convergence rates with respect to the assumed regularity of Ψ in μ and θ.

Lemma 4.1. *Let $e_J[\Psi]$ denote the error in* (4.5)*, with J equally spaced quadrature points $\theta_j \in [0, 2\pi]$. Suppose that $\left|\frac{\partial^r\Psi(\mathbf{x},\mu,\theta)}{\partial\theta^r}\right|$ is integrable on $[0, 2\pi]$, then*

$$|e_J[\Psi]| \leq \frac{C_r}{J^r}\int_0^{2\pi}\Big|\frac{\partial^r\Psi(\mathbf{x},\mu,\theta)}{\partial\theta^r}\Big|d\theta, \tag{4.7}$$

where C_r is independent of J and Ψ.

Lemma 4.2. *Let $e_K[\Psi]$ denote the error in K-point Gaussian quadrature approximation of the integral of Ψ on $\mu \in [-1,1]$. Suppose that $(1-\mu^2)^{s/2}\Big|\frac{\partial^s\Psi(\mathbf{x},\mu,\theta)}{\partial\mu^s}\Big|$ is integrable on $[-1,1]$, then*

$$|e_K[\Psi]| \le \frac{C_s}{K^s}\int_{-1}^{1}\Big|\frac{\partial^s\Psi(\mathbf{x},\mu,\theta)}{\partial\mu^s}\Big|\cdot(1-\mu^2)^{s/2}\,d\mu, \tag{4.8}$$

where C_s is independent of K and Ψ.

We postpone the proofs of these lemmas and first derive the proof of Theorem 3.2 from them. For the transport equation (3.1), in polygonal domains, the regularity requirements in the lemmas 4.1 and 4.2 are proved for $r = s = 1$ in [1]:

Proposition 4.3. *Let $\frac{\partial\Psi}{\partial\theta} \in L_1[0,2\pi]$ and $\frac{\partial\Psi}{\partial\mu} \in L_1^{\tilde{w}}[-1,1]$, where $\tilde{w} := (1-\mu^2)^{1/2}$. Then for the quadrature error $\tau(\mathbf{x})$ of the approximation (4.3) we have,*

$$\|\tau\|_{L_2(\Omega)} \le C\Big(\frac{1}{J}+\frac{1}{K}\Big)\|g\|_{H^1(\Omega)}, \tag{4.9}$$

where g is the right hand side of (3.1), i.e., $g = \sigma_s\tilde{\Psi} + S$ with $\tilde{\Psi} = \int_{-1}^{1}\int_0^{2\pi}\Psi$, and $H^1(\Omega)$ is the usual L_2-based Sobolev space of order one on Ω.

Now we are ready to derive our final error estimate:

Proof of Theorem 3.2. We multiply (3.10) by $\frac{T_k(y)}{\sqrt{1-y^2}}$, $k = 0,\dots,L$, integrate over $y \in [-1,1]$ and use the Cauchy-Schwarz inequality to get for $l = 0,\dots,L$,

$$\begin{aligned}
\tau^l(x) &= \frac{2-\delta_{l,0}}{\pi}\int_{-1}^{1}\tau(\mathbf{x})\frac{T_l(y)}{\sqrt{1-y^2}}\,dy\\
&\le \frac{2-\delta_{l,0}}{\pi}\Big(\int_{-1}^{1}\tau(\mathbf{x})^2\,\frac{dy}{\sqrt{1-y^2}}\Big)^{1/2}\Big(\int_{-1}^{1}T_l(y)^2\,\frac{dy}{\sqrt{1-y^2}}\Big)^{1/2}\\
&= \Big(\frac{2-\delta_{l,0}}{\pi}\int_{-1}^{1}\tau(\mathbf{x})^2\,\frac{dy}{\sqrt{1-y^2}}\Big)^{1/2}.
\end{aligned} \tag{4.10}$$

Now recalling (3.12) it follows that

$$\|\tau^l\| \le \frac{2-\delta_{l,0}}{\pi}\Big(\int_{-1}^{1}\int_{-1}^{1}\tau(\mathbf{x})^2\,\frac{dy}{\sqrt{1-y^2}}\,dx\Big)^{1/2} \le C\,\|\tau\|_{L_2(\Omega)}. \tag{4.11}$$

Combining with (4.9), recalling also $M \sim J^{1/2} \sim K^{1/2}$ we get the desired result. □

Remark. The convergence rate in Lemmas 4.1 and 4.2, as well as the rates in Proposition 4.3, can be improved up to the optimal order $\mathcal{O}(J^{2-\varepsilon}) \sim \mathcal{O}(K^{2-\varepsilon})$, ε arbitrarily small, for the neutron transport equation, in polygonal domains using, e.g., a post processing procedure cf. Asadzadeh [2].

Now it remains to verify the estimates in Lemmas 4.1-4.2.

Proof of Lemma 4.1. We may assume that Ψ is 2π-periodic in θ and in the quadrature formula

$$\int_0^{2\pi}\Psi(\mathbf{x},\mu,\theta)d\theta \sim \sum_{j=1}^{J}W_j\Psi(\mathbf{x},\mu,\theta_j), \tag{4.12}$$

approximate Ψ by trigonometric polynomials in θ. Then we can easily check that: no matter how we choose the quadrature points θ_j and weights W_j, the formula (4.12) can not be exact for trigonometric polynomials of degree J, (see, e.g., [13] for the details). It turns out that the highest degree of precision $J-1$ is achieved just for our simplest quadrature formula: equally spaced nodes $\theta_j = \frac{2\pi j}{J}$ and constant weights $W_j = \frac{2\pi}{J}$, $j = 1, 2, \dots, J$. Thus we have

$$\int_0^{2\pi} \Psi(\theta) d\theta \sim \frac{2\pi}{J} \sum_{j=1}^{J} \Psi\Big((j-1)\frac{2\pi}{J}\Big). \tag{4.13}$$

We can easily verify that (4.13) is exact for the functions $e^{imx}, m = 0, 1, \dots, J-1$. Further a trigonometric polynomial of degree J, with the Fourier series expansion

$$T_J(x) \equiv \frac{a_0}{2} + \sum_{j=1}^{J} (a_j \cos jx + b_j \sin jx), \tag{4.14}$$

having $2J+1$ degrees of freedom (a_0, a_j, b_j, $j = 1, \dots, J$) corresponds to an algebraic polynomials of degree $2J$. Thus (4.13) is exact for algebraic polynomials of degree $2J-1$, so that for $\Psi \in C^{(r)}[0, 2\pi]$, $r = 2J$, (Ψ is $2J$ times continuously differentiable in θ), using Taylor expansion up to degree $2J-1$, in both sides of (4.12), we obtain the desired result. $\square$

Lemma 4.2 is a special case of the a classical result due to DeVore and Scott (Theorem 3 in [8], Proposition 4.4 below): Consider, for positive integer s, the function space

$$\Psi \in Y_w^s := \{u \in L^1_{loc}(]-1,1[) : \|u\|_{w,s} < \infty\} \tag{4.15}$$

with w being a weight function and

$$\|u\|_{w,s} = \int_{-1}^{1} [|u(\mu)| + |u^{(s)}(\mu)|(1-\mu^2)^s] w(\mu)\, d\mu, \tag{4.16}$$

where $u^{(s)}$ is interpreted as a weak derivative.

Proposition 4.4 (DeVore and Scott). *Let $e_K[\Psi]$ denote the error in K-point Gaussian quadrature approximation of the integral of Ψ on $[-1,1]$. Suppose that $(1-\mu^2)^s \left|\frac{\partial^s \Psi(\mathbf{x},\mu,\theta)}{\partial \mu^s}\right|$ (weak derivative) is integrable on $[-1,1]$, i.e., $\Psi \in Y_1^s$, where s is any positive integer such that $1 \le s \le 2K$. Then*

$$|e_K[\Psi]| \le C_s \int_{-1}^{1} \Big|\frac{\partial^s \Psi(\mathbf{x},\mu,\theta)}{\partial \mu^s}\Big| \min\Big\{\Big(\frac{\sqrt{1-\mu^2}}{K}\Big)^s, (1-\mu^2)^s\Big\}\, d\mu, \tag{4.17}$$

where C_s is independent of K and Ψ.

Proof of Lemma 4.2. This follows, evidently, from the Proposition 4.4. $\square$

Below we review a procedure, based on analyzing the Peano kernel for the quadrature error (4.6), and establish the bound (4.8) for $s = 1$, see [1] or [8]. This would suffices to justify the use of Proposition 4.3. The full proof of (4.8), or (4.17), for $s \ge 1$ is treated as in [8]. Consider the Gauss quadrature rule

$$\int_{-1}^{1} \Psi(\mathbf{x};\mu,\theta) d\mu \sim \sum_{k=1}^{K} A_k \Psi(\mathbf{x},\mu_k,\theta), \tag{4.18}$$

where

$$\mu_k := -\cos\alpha_k, \quad \alpha_k \in \Big[\frac{(2k-1)\pi}{2K+1}, \frac{2k\pi}{2K+1},\Big], \quad k = 1, \dots, K, \tag{4.19}$$

are zeros of Legendre polynomials and

$$A_k := \int_{-1}^{1} \prod_{l \neq k} \frac{x - x_l}{x_k - x_l}\, dx, \quad k = 1, \dots, K, \tag{4.20}$$

are the integrals of the associated Lagrange interpolation polynomials. Now using the Peano kernel theorem we can write

$$e_K[\Psi] = \int_{-1}^{1} \Lambda(\zeta)\Psi'(\zeta)\, d\zeta, \tag{4.21}$$

where $\Lambda(\zeta) = e_K[H_\zeta]$, $|\zeta| \leq 1$ and H_ζ is the Heaviside function

$$H_\zeta(\mu) := \begin{cases} 0, & \mu < \zeta, \\ 1, & \mu \geq \zeta. \end{cases} \tag{4.22}$$

It follows that

$$\Lambda(\zeta) = 1 - \zeta - \sum_{\mu_k > \zeta} A_k = \sum_{\mu_k < \zeta} A_k - \zeta - 1. \tag{4.23}$$

By the Chebyshev-Markov-Stieltjes (cf. [17] p. 50) inequality we have

$$1 + \mu_k \leq \sum_{i=1}^{k} A_i \leq 1 + \mu_{k+1}, \quad k = 1, \dots, K. \tag{4.24}$$

Thus with $-1 = \mu_0 < \mu_1 < \ldots < \mu_K < \mu_{K+1} = 1$ we get for $k = 1, \dots, K$ that

$$\mu_{k-1} - \mu_k \leq \Lambda(\mu_k-) \leq 0 \leq \Lambda(\mu_k+) \leq \mu_{k+1} - \mu_k. \tag{4.25}$$

Since Λ vanishes on each interval $[\mu_{k-1}, \mu_k]$ and has the slope one almost everywhere, we have

$$\max\{|\Lambda(\mu)| : \mu \in [\mu_{k-1}, \mu_k]\} \leq \mu_k - \mu_{k-1}, \quad k = 1, \dots, K. \tag{4.26}$$

To bound $\mu_k - \mu_{k-1}$, we define $I_k := [\alpha_{k-1}, \alpha_k]$, then

$$\begin{aligned} \mu_k - \mu_{k-1} = \cos\alpha_{k-1} - \cos\alpha_k &= \int_{\alpha_{k-1}}^{\alpha_k} \sin\alpha\, d\alpha \\ &\leq (\alpha_k - \alpha_{k-1}) \max_{\alpha \in I_k}\{\sin\alpha\} \leq \frac{3\pi}{2K} \max_{\alpha \in I_k}\{\sin\alpha\}. \end{aligned} \tag{4.27}$$

Now since $(\sin\alpha)/\alpha$ is decreasing in $[0, \pi]$, using (4.19) we get

$$\sin\alpha \leq \Big(\frac{\alpha}{\alpha_{k-1}}\Big) \sin\alpha_{k-1} \leq \Big(\frac{\alpha_k}{\alpha_{k-1}}\Big) \sin\alpha_{k-1} \leq 4\sin\alpha_{k-1}, \quad \alpha \in I_k, \tag{4.28}$$

for $k = 2, \dots, K$. By the symmetry properties of α_j (cf. [17]) we also get

$$\sin\alpha \leq 4\sin\alpha_k, \quad \alpha \in I_k, \qquad k = 2, \dots, K. \tag{4.29}$$

Thus for $k = 2, \dots, K$,

$$\max_{\alpha \in I_k}\{\sin\alpha\} \leq 4 \min_{\alpha \in I_k}\{\sin\alpha\} \equiv 4 \min_{\alpha \in I_k}\{\sqrt{1 - \cos^2\alpha}\}. \tag{4.30}$$

Hence, combining (4.27) and (4.30), and using (4.19) we have for $k = 2, \dots, K$,

$$\mu_k - \mu_{k-1} = \frac{6\pi}{K} \min_{\alpha \in I_k} \{\sqrt{1-\cos^2\alpha}\} = \frac{6\pi}{K} \min_{\alpha \in I_k} \{\sqrt{1-\mu^2}\}. \tag{4.31}$$

Thus, by (4.26), for $\mu \in [\mu_1, \mu_N]$,

$$|\Lambda(\mu)| \leq \frac{6\pi\sqrt{1-\mu^2}}{K}. \tag{4.32}$$

The corresponding estimate for $\mu \in [-1, \mu_1]$ and $\mu \in [\mu_N, 1]$ is (see [8]):

$$|\Lambda(\mu)| \leq \frac{\pi\sqrt{1-\mu^2}}{\sqrt{2}K}. \tag{4.33}$$

Summing up we have shown

$$|e_K[\Psi]| \leq \frac{6\pi}{K} \int_{-1}^{1} \left|\frac{\partial \Psi}{\partial \mu}\right| \cdot \sqrt{1-\mu^2}\, d\mu. \tag{4.34}$$

This proves (4.8) for $s = 1$. For further details we refer to [1] and [8].

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5. Appendix I: Elementary properties of Chebyshev Polynomials

Chebyshev polynomials are weighted orthogonal polynomials defined by

$$T_n(x) = \cos(n \arccos(x)), \tag{5.1}$$

with the weight function $w(x) = \frac{1}{\sqrt{1-x^2}}$. Thus Chebeshev polynomials are a subclass of Jacobi polynomials, where the Jacobi weights $w_J = (1+x)^a(1-x)^b$, $a, b > -1$ are restricted to $a = b = -1/2$. It follows that

$$\int_{-1}^{1} T_i(x)T_j(x)w(x)\,dx = \begin{cases} 0 & i \neq j \\ \pi/2 & i = j \neq 0 \\ \pi & i = j = 0. \end{cases} \tag{5.2}$$

Hence

$$\|T_i\|_w = \frac{\pi}{2-\delta_{i,0}}, \qquad i = 0, 1, \ldots. \tag{5.3}$$

$T_n(x)$ is a polynomial of degree n, orthogonal to all polynomials of degree $\leq n-1$. On differentiating $T_n(x) = \cos n\beta$ with respect to $x(=\cos\beta)$ we obtain a polynomial of degree $n-1$ called *the Chebyshev polynomials of second kind:*

$$U_{n-1} = \frac{1}{n}T_n'(x) = \frac{\sin n\beta}{\sin\beta}, \qquad x = \cos\beta. \tag{5.4}$$

Further we can easily verify the following properties (see [15] for the details):
For even (odd) n only even (odd) powers of x occur in $T_n(x)$.

$$T_n(-x) = (-1)^n T_n(x). \tag{5.5}$$

$$\frac{1}{2} + T_2(x) + T_4(x) + \ldots + T_{2k}(x) = \frac{U_{2k}(x)}{2}, \qquad k = 0, 1, \ldots, \tag{5.6}$$

$$T_1(x) + T_3(x) + \ldots + T_{2k+1}(x) = \frac{U_{2k+1}(x)}{2}, \qquad k = 0, 1, \ldots,. \tag{5.7}$$

Below we formulate and prove the property that has been essential in deriving the basic estimate in section 3 (Proposition 3.4.):

Proposition 5.1. *Let*

$$\gamma_j(l) := \int_{-1}^{1} \frac{d}{dy}T_l(y) \cdot \frac{T_j(y)}{\sqrt{1-y^2}}\,dy, \tag{5.8}$$

we have that

$$\gamma_j(l) = 0, \qquad for \quad j \geq l, \tag{5.9}$$

and for $j < l$,

$$\gamma_j(l) = \begin{cases} 0, & j+l \quad even \\ l\pi, & j+l \quad odd. \end{cases} \tag{5.10}$$

Proof. The first assertion is a trivial consequence of the fact that T_j is orthogonal to all polynomials of degree $\leq j-1$. As for the second assertion we note that

$$T_l'(x) = lU_{l-1}(x).$$

Thus if l is odd then $l-1$ is even, say $l-1=2k$, hence using (5.6)

$$\begin{aligned}\gamma_j(l) &= 2l\int_{-1}^{1}\Big[\frac{1}{2}+T_2(x)+T_4(x)+\ldots+T_{l-1}(x)\Big]\cdot\frac{T_j(y)}{\sqrt{1-y^2}}\,dy \\ &= \begin{cases} 0, & j \text{ odd, i.e., } j+l \text{ even} \\ 2l\frac{\pi}{2-\delta_{j,0}}, & j \text{ even, i.e., } j+l \text{ odd.}\end{cases}\end{aligned} \tag{5.11}$$

The case l is even is treated similarly and using (5.7) and the proof is complete. □

6. Appendix II: The three-dimensional spectral solution

We extend now the approach presented in Section 2 to the transport process in three dimensions,

$$\begin{aligned}&\mu\frac{\partial}{\partial x}\Psi(\mathbf{x},\mu,\theta)+\sqrt{1-\mu^2}\left(\cos\theta\frac{\partial}{\partial y}\Psi(\mathbf{x},\mu,\theta)+\sin\theta\frac{\partial}{\partial z}\Psi(\mathbf{x},\mu,\theta)\right)\\ &+\sigma_t\Psi(\mathbf{x},\mu,\theta)=\int_{-1}^{1}\int_0^{2\pi}\sigma_s(\mu',\theta'\to\mu,\theta)\Psi(\mathbf{x},\mu',\theta')d\theta' d\mu'+S(\mathbf{x},\mu,\theta),\end{aligned} \tag{6.1}$$

where we assume that the spatial variable $\mathbf{x}:=(x,y,z)$ varies in the cubic domain $\Omega:=\{(x,y,z): -1\leq x,\,y,\,z\leq 1\}$, and $\Psi(\mathbf{x},\mu,\theta):=\Psi(x,y,z,\mu,\theta)$ is the angular flux in the directions defined by $\mu\in[-1,1]$ and $\theta\in[0,2\pi]$.

We seek for a solution of (6.1) satisfying the following boundary conditions: For the boundary terms in x; for $0\leq\theta\leq 2\pi$,

$$\Psi(x=\pm1,y,z,\mu,\theta)=\begin{cases} f_1(y,z,\mu,\theta), & x=-1, \quad 0<\mu\leq 1,\\ 0, & x=1, \quad -1\leq\mu<0,\end{cases} \tag{6.2}$$

For the boundary terms in y and for $-1<\mu<1$,

$$\Psi(x,y=\pm1,z,\mu,\theta)=\begin{cases} f_2(x,z,\mu,\theta), & y=-1, \quad 0<\cos\theta\leq 1,\\ 0, & y=1, \quad -1\leq\cos\theta<0.\end{cases} \tag{6.3}$$

Finally, for the boundary terms in z; for $-1<\mu<1$,

$$\Psi(x,y,z=\pm1,\mu,\theta)=\begin{cases} f_3(x,y,\mu,\theta), & z=-1, \quad 0\leq\theta<\pi,\\ 0, & z=1, \quad \pi<\theta\leq 2\pi.\end{cases} \tag{6.4}$$

Here we assume that $f_1(y,z,\mu,\theta)$, $f_2(x,z,\mu,\theta)$ and $f_3(x,y,\mu,\theta)$ are given functions.

Expanding the angular flux $\Psi(x,y,z,\mu,\theta)$ in a truncated series of Chebyshev polynomials $T_i(y)$and $R_j(z)$ leads to

$$\Psi(x,y,z,\mu,\theta)=\sum_{i=0}^{I}\sum_{j=0}^{J}\Psi_{i,j}(x,\mu,\theta)T_i(y)R_j(z). \tag{6.5}$$

We repeat the procedure in Section 2 and insert $\Psi(x,y,z,\mu,\theta)$ given by (6.5) into the boundary conditions in (6.3), for $y=\pm1$. Multiplying the resulting expressions by $\frac{Rj(z)}{\sqrt{1-z^2}}$ and integrating over z, we get the components $\Psi_{0,j}(x,\mu,\theta)$, $j=0,\ldots,J$:

$$\Psi_{0,j}(x,\mu,\theta)=f_2^j(x,\mu,\theta)-\sum_{i=1}^{I}(-1)^i\Psi_{i,j}(x,\mu,\theta), \qquad 0<\cos\theta\leq 1, \tag{6.6}$$

and

$$\Psi_{0,j}(x,\mu,\theta) = -\sum_{i=1}^{I} \Psi_{i,j}(x,\mu,\theta), \qquad -1 \le \cos\theta < 0. \tag{6.7}$$

Similarly, we substitute $\Psi(x,y,z,\mu,\theta)$ from (6.5) into the boundary conditions for $z=\pm 1$, multiply the resulting expressions by $\frac{T_i(y)}{\sqrt{1-y^2}}$, $i=1,\dots,I$ and integrate over y, to define the components $\Psi_{i,0}(x,\mu,\theta)$, $i=0,\dots,I$: For $-1\le x\le 1,\ -1<\mu<1$,

$$\Psi_{i,0}(x,\mu,\theta) = f_3^i(x,\mu,\theta) - \sum_{j=1}^{J}(-1)^j \Psi_{i,j}(x,\mu,\theta), \qquad 0 \le \theta < \pi, \tag{6.8}$$

$$\Psi_{i,0}(x,\mu,\theta) = -\sum_{j=1}^{J} \Psi_{i,j}(x,\mu,\theta), \qquad \pi < \theta \le 2\pi, \tag{6.9}$$

where

$$f_2^j(x,\mu,\theta) = \frac{2-\delta_{0,j}}{\pi}\int_{-1}^{1} f_2(x,z,\mu,\theta)\frac{R_j(z)}{\sqrt{1-z^2}}dz \tag{6.10}$$

and

$$f_3^i(x,\mu,\theta) = \frac{2-\delta_{i,0}}{\pi}\int_{-1}^{1} f_3(x,y,\mu,\theta)\frac{T_i(y)}{\sqrt{1-y^2}}dy. \tag{6.11}$$

To determine the components $\Psi_{i,j}(x,\mu,\theta)$, $i=1,\dots,I$, and $j=1,\dots,J$, we substitute $\Psi(x,\mu,\theta)$, from (6.5) into (6.1) and the boundary conditions for $x=\pm 1$. Multiplying the resulting expressions by $\frac{T_i(y)}{\sqrt{1-y^2}} \times \frac{R_j(z)}{\sqrt{1-z^2}}$, and integrating over y and z we obtain $I\times J$ one-dimensional transport problems, viz

$$\begin{aligned} \mu\frac{\partial\Psi_{i,j}}{\partial x}(x,\mu,\theta) + \sigma_t\Psi_{i,j}(x,\mu,\theta) &= G_{i,j}(x;\mu,\theta) \\ &+ \int_{-1}^{1}\int_{-1}^{1}\sigma_s(\mu',\theta' \to \mu,\theta)\Psi_{i,j}(x,\mu',\theta')d\theta' d\mu', \end{aligned} \tag{6.12}$$

with the boundary conditions

$$\Psi_{i,j}(-1,\mu,\theta) = f_1^{i,j}(\mu,\theta), \tag{6.13}$$

where

$$f_1^{i,j}(\mu,\theta) = \frac{4}{\pi^2}\int_{-1}^{1}\int_{-1}^{1}\frac{T_i(y)R_j(z)}{\sqrt{(1-y^2)(1-z^2)}} f_1(y,z,\mu,\theta)dzdy, \tag{6.14}$$

and

$$\Psi_{i,j}(1,-\mu,\theta) = 0, \tag{6.15}$$

for $0<\mu\le 1$, and $0\le\theta\le 2\pi$. Finally

$$\begin{aligned} G_{i,j}(x,\mu,\theta) &= S_{i,j}(x,\mu,\theta) - \\ &\sqrt{1-\mu^2}\times\left[\cos\theta\sum_{k=i+1}^{I} A_i^k\Psi_{k,j}(x,\mu,\theta) + \sin\theta\sum_{l=j+1}^{J} B_j^l\Psi_{i,l}(x,\mu,\theta)\right], \end{aligned} \tag{6.16}$$

with

$$S_{i,j}(x,\mu,\theta) = \frac{4}{\pi^2}\int_{-1}^{1}\int_{-1}^{1}\frac{T_i(y)R_j(z)}{\sqrt{(1-y^2)(1-z^2)}}S(\mathbf{x},\mu,\theta)dzdy, \tag{6.17}$$

$$A_i^k = \frac{2}{\pi}\int_{-1}^{1}\frac{d}{dy}(T_k(y))\frac{T_i(y)}{\sqrt{1-y^2}}\,dy \tag{6.18}$$

$$B_j^l = \frac{2}{\pi}\int_{-1}^{1}\frac{d}{dz}(R_l(z))\frac{R_j(z)}{\sqrt{1-z^2}}\,dz. \tag{6.19}$$

Now, starting from the solution of the problem given by equations (6.12)–(6.19) for $\Psi_{I,J}(x,\mu,\theta)$, we then solve the problems for the other components, in the decreasing order in i and j. Recall that $\sum_{i=I+1}^{I}\cdots = \sum_{j=J+1}^{J}\cdots \equiv 0$. Hence, solving $I\times J$ one-dimensional problems, the angular flux $\Psi(\mathbf{x},\mu,\theta)$, is now completely determined through (6.5).

Remark: If we have to deal with a different type of boundary conditions, we have to keep in mind that the first components $\Psi_{i,0}(x,\mu,\theta)$ and $\Psi_{0,j}(x,\mu,\theta)$ are determined from the boundary conditions for z and y and the other ones, $\Psi_{i,j}(x,\mu,\theta)$ for $i = 1,\dots,I$ and $j = 1,\dots,J$ will satisfy one-dimensional transport problems subject to the same type of boundary conditions of the original problem in the variable x.

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