On the eigenstructure of spherical harmonic equations for radiative transport

C. Kristopher Garrett*, Cory D. Hauck†

July 10, 2015

Abstract

The spherical harmonic equations for radiative transport are a linear, hyperbolic set of balance laws that describe the state of a system of particles as they advect through and collide with a material medium. For regimes in which the collisionality of the system is light to moderate, significant qualitative differences have been observed between solutions, based on whether the angular approximation used to derive the equations occurs in a subspace of even or odd degree. This difference can be traced back to the eigenstructure of the coefficient matrices in the advection operator of the hyperbolic system. In this paper, we use classical properties of the spherical harmonics to examine this structure. In particular, we show how elements in the null space of the coefficient matrices depend on the parity of the spherical harmonic approximation and we relate these results to observed differences in even and odd expansions.

1 Introduction

The spherical harmonic equations are a set of linear, Hermitian hyperbolic balance laws that model radiation transport through a material medium. For a purely scattering material (no absorption and no sources) and an infinite medium, the time dependent version of these equations for the vector-valued unknown $\mathbf{u}\colon \mathbb{R}^3 \times \mathbb{R}^{\geq 0} \to \mathbb{C}^n$ is

$$\begin{cases} \partial_t \mathbf{u}(x,t) + \sum_{i=1}^{3} \mathbf{A}_i \partial_{x_i} \mathbf{u}(x,t) + \sigma_{\mathrm{s}}(x) \mathbf{Q} \mathbf{u}(x,t) = 0\,, & (x,t) \in \mathbb{R}^3 \times \mathbb{R}^{>0} \\ \mathbf{u}(x,0) = \mathbf{u}_0(x)\,, & x \in \mathbb{R}^3 \end{cases} . \tag{1}$$

Here the initial condition $\mathbf{u}_0$ is given; the matrices $\mathbf{A}_i$ are constant and Hermitian; $\mathbf{Q}$ is a constant diagonal matrix with non-negative entries; and the non-negative coefficient $\sigma_{\mathrm{s}}(x)$ is the scattering cross-section.

The kinetic interpretation (1) is straightforward. Let $f\colon \mathbb{R}^3 \times \mathbb{S}^2 \times \mathbb{R}^{\geq 0} \to \mathbb{R}^{\geq 0}$, where $\mathbb{S}^2$ is the unit sphere in $\mathbb{R}^3$, be the solution of the linear kinetic equation

$$\begin{cases} \partial_t f(x,\Omega,t) + \Omega \cdot \nabla_x f(x,\Omega,t) + \sigma_{\mathrm{s}}(x) \mathcal{Q} f(x,\Omega,t) = 0\,, & (x,\Omega,t) \in \mathbb{R}^3 \times \mathbb{S}^2 \times \mathbb{R}^{>0} \\ f(x,\Omega,0) = f_0(x,\Omega)\,, & (x,\Omega) \in \mathbb{R}^3 \times \mathbb{S}^2 \end{cases} . \tag{2}$$

Here $\mathcal{Q}$, which models particle scattering at the kinetic level, is an integral operator in Ω at each (x,t); for any function $h\colon \mathbb{S}^2 \to \mathbb{R}$,

$$(\mathcal{Q}h)(\Omega) = h(\Omega) - \int_{\mathbb{S}^2} g(\Omega \cdot \Omega') h(\Omega') d\Omega'\,, \tag{3}$$

*Computer Science and Mathematics Division, Oak Ridge National Laboratory, `garrettck@ornl.gov`

†Computer Science and Mathematics Division, Oak Ridge National Laboratory and Department of Mathematics, University of Tennessee, `hauckc@ornl.gov`

where g is a bounded probability distribution on $[-1,1]$.

Let $\theta \in [0,\pi)$ and $\varphi \in [0,2\pi)$ be polar and azimuthal angles on the sphere so that, in Cartesian coordinates, $\Omega = (\Omega_1, \Omega_2, \Omega_3) = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$. For any integer $\ell \geq 0$, let $\mathbf{Y}_\ell \colon \mathbb{S}^2 \to \mathbb{C}^{2\ell+1}$ be a vector-valued function whose components are the $2\ell+1$ spherical harmonics of degree ℓ (we abuse notation and let $Y_\ell^m(\theta,\varphi) = Y_\ell^m(\Omega)$):

$$Y_\ell^k(\theta,\varphi) = \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-k)!}{(\ell+k)!}}\, P_\ell^k(\cos\theta)\, e^{ik\varphi}\,, \quad |k| \leq \ell\,, \tag{4}$$

where P_ℓ^k is an associated Legendre function:

$$P_\ell^k(\mu) = \begin{cases} (1-\mu^2)^{k/2}\dfrac{d^k P_\ell}{d\mu^k}(\mu), & k \geq 0 \\ \\ (-1)^k \frac{(\ell+k)!}{(\ell-k)!} P_\ell^{-k}(\mu), & k < 0, \end{cases} \tag{5}$$

and $P_\ell \colon [-1,1] \to \mathbb{R}$ is the degree ℓ Legendre polynomial, normalized such that $\int_{-1}^1 |P_\ell|^2 = 2/(2\ell+1)$.

Given a fixed positive integer N, set $\mathbf{Y} = [\mathbf{Y}_0^T, \ldots, \mathbf{Y}_N^T]^T$. Then $\mathbf{Y} \colon \mathbb{S}^2 \to \mathbb{C}^n$, where $n = \sum_{\ell=0}^N 2\ell + 1 = (N+1)^2$. The spherical harmonic approximation of f is given by

$$f_N(x,\Omega,t) := \mathbf{Y}^H(\Omega)\mathbf{u}(x,t) = \sum_{\ell=0}^N \mathbf{Y}_\ell^H(\Omega)\mathbf{u}_\ell(x,t) = \sum_{\ell=0}^N \sum_{|k|\leq\ell} \overline{Y_\ell^k}(\Omega) u_\ell^k(x,t)\,, \tag{6}$$

where $\mathbf{u} = \langle \mathbf{Y} f_N \rangle$ satisfies (1), with $\mathbf{A}_i$ and $\mathbf{Q}$ given by

$$\mathbf{A}_i = \left\langle \Omega_i \mathbf{Y}\mathbf{Y}^H \right\rangle \quad \text{and} \quad \mathbf{Q} = \left\langle \mathbf{Y}(\mathcal{Q}\mathbf{Y}^H) \right\rangle\,, \tag{7}$$

where $\mathcal{Q}\mathbf{Y}^H$ is evaluated component by component, and we have adopted the shorthand notation $\langle \cdot \rangle := \int_{\mathbb{S}^2} (\cdot)\, d\Omega$. Here $\mathbf{Y}^H$ is the conjugate transpose of $\mathbf{Y}$, and we have adopted for $\mathbf{u}$ the natural indexing for the spherical harmonics, namely $\mathbf{u} = [\mathbf{u}_0^T, \ldots, \mathbf{u}_N^T]^T$, where for each ℓ, $\mathbf{u}_\ell = [u_\ell^{-\ell}, \ldots, u_\ell^0, \ldots, u_\ell^\ell]^T$. Because f is a real-valued function, the number of independent components in $\mathbf{u}$ is only $(N+1)^2$. Indeed, since $\overline{Y_\ell^k} = (-1)^k Y_\ell^{-k}$, it follows that $u_\ell^k := \langle Y_\ell^k f_N \rangle = (-1)^k \langle \overline{Y_\ell^{-k}} f_N \rangle = (-1)^k \overline{u_\ell^{-k}}$.

The matrices $\mathbf{A}_i$ can be computed using the following recursion relations to expand $\Omega_i \mathbf{Y}$ in terms of spherical harmonics [2]:

$$\Omega Y_\ell^k = \frac{1}{2} \begin{bmatrix} -c_{\ell-1}^{k-1} Y_{\ell-1}^{k-1} + d_{\ell+1}^{k-1} Y_{\ell+1}^{k-1} + e_{\ell-1}^{k+1} Y_{\ell-1}^{k+1} - f_{\ell+1}^{k+1} Y_{\ell+1}^{k+1} \\ i\left(c_{\ell-1}^{k-1} Y_{\ell-1}^{k-1} - d_{\ell+1}^{k-1} Y_{\ell+1}^{k-1} + e_{\ell-1}^{k+1} Y_{\ell-1}^{k+1} - f_{\ell+1}^{k+1} Y_{\ell+1}^{k+1} \right) \\ 2(a_{\ell-1}^k Y_{\ell-1}^k + b_{\ell+1}^k Y_{\ell+1}^k) \end{bmatrix}\,, \tag{8}$$

where the nonzero recursion coefficients are known, see [2], and we set $Y_\ell^k \equiv 0$ for $\ell < 0$ and $|k| > \ell$. The relations in (8) follow directly from well-known recursion formulas for the associated Legendre functions; see, for example, [1]. The matrix $\mathbf{Q}$, on the other hand, is found by expanding g in Legendre polynomials and applying the additional formula for spherical harmonics. See, for example [12, Appendix A].

We focus in this paper on the structure of the matrices $\mathbf{A}_i$; the specific values of the matrix elements will not be necessary. The values of the matrix elements in $\mathbf{Q}$ are also not necessary.

2 Difference between N odd and N even

In practice, the spherical harmonic equations are rarely applied with even values of N. Most of the discussion in the literature on this point refers to the reduced equations in a slab geometry. In this case, many of the elements of $\mathbf{u}$ are identically zero, but the equations for the $N+1$ nonzero elements again form a hyperbolic balance law in one dimension with a single flux matrix $\mathbf{A}$. (See for example [14, Section 3.5], [12, Appendix D], [4, Section 8.4], [6, Chapter 10], or [11, Section 2.1].) The disadvantages of even N in slab geometry are noted, somewhat in passing, in [4, 12, 14]. To our knowledge, the most substantial (although somewhat dated) presentation, which includes some of the discussion below, can be found in [6, Chapter 10].

For N odd, the eigenvalues of $\mathbf{A}$ appear in pairs that differ only by sign; for N even, they also appear in signed pairs, except for a single zero eigenvalue. This zero eigenvalue means that for steady-state equations in a void ($\sigma_\mathrm{s} = 0$), the system has an infinite number of solutions and is therefore not well-posed. In addition, the specification of well-posed boundary conditions is more complicated: any strong-form prescription which treats both ends of the slab in the same way leads to an even number of boundary conditions. Therefore, unless chosen very specifically, the boundary conditions will be either under or over-specified. Finally, enforcing continuity of f across material interfaces (discontinuities in σ_s) leads to unique interface conditions on the moments only for odd N. For even N, an additional ad-hoc condition is required.

For the multidimensional case, we are aware of even less discussion in the literature. While the results for the slab geometry case are still relevant, it turns out that each of the matrices $\mathbf{A}_i$ has (multiple) zero eigenvalues for both N even and odd, making the steady-state equations in a void ill-posed. A finite element version of the spherical harmonic equations can be formulated directly from the original kinetic equation, imposing boundary conditions weakly. For $\sigma_\mathrm{s} > 0$ it is possible to define a bilinear form which leads to a well-posed problem for both N odd and even. See, for example [7, 13]. However, when σ_s vanishes, the finite element formulation requires certain properties between even and odd test spaces which are not satisfied by the spherical harmonic formulation [8].

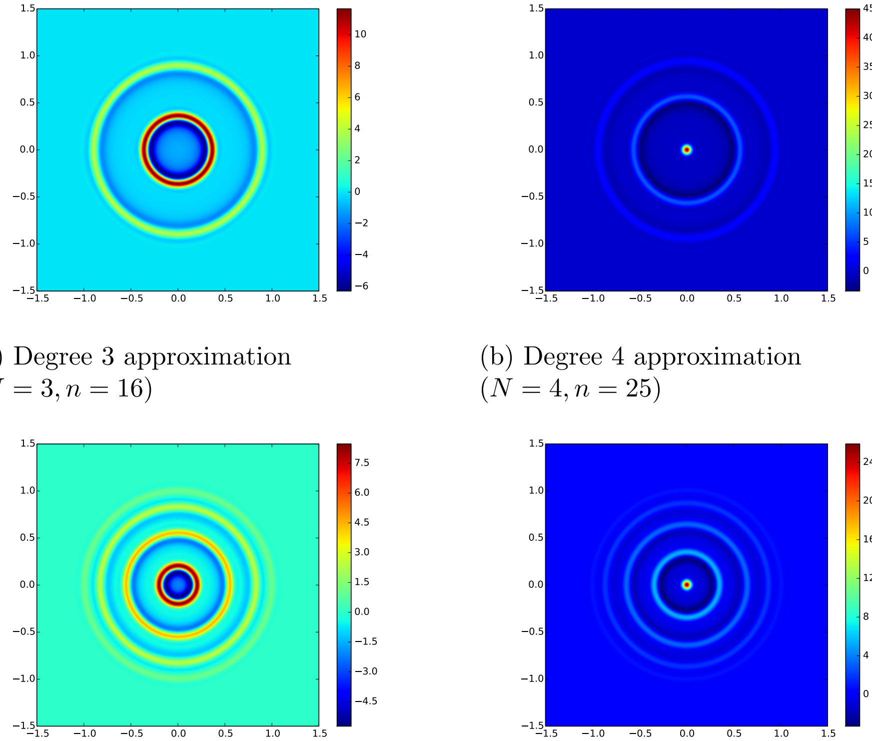
For low-order solutions (N small) with little scattering, the even and odd cases exhibit distinctly different wave behavior, even for the whole-space problem (1) with no boundary conditions or internal interfaces. We demonstrate these differences using the so-called linesource benchmark, which was designed in [9] and has since been used to study the performance of various approximation methods for (2) [3, 10]. The problem involves an initial particle source concentrated on an infinite line in $\mathbb{R}^3$. The symmetry of the problem allows it to be formulated in a reduced two-dimensional geometry. The initial source is represented mathematically by the initial condition

$$f_0(x, y, \Omega_1, \Omega_2, \Omega_3) = \frac{1}{4\pi}\delta(x, y) \tag{9}$$

and $\sigma_s = 0$. Numerical results for several values of N are given in Figure 1.[1] In all cases, we observe wave-like behavior. However, only for even N do we see that a significant fraction of the mass remains very near the origin.

A brief explanation for the differences observed in Figure 1 is given in [2, Section 2.2] based on the eigenstructure of $\mathbf{A}_1$, $\mathbf{A}_2$, and $\mathbf{A}_3$. There, it is noted that for even N, there is an eigenvector

[1] To reduce spatial grid effects, we use a sharp Gaussian with a standard deviation of 0.03 to approximate the initial condition.



(a) Degree 3 approximation
$(N = 3, n = 16)$

(b) Degree 4 approximation
$(N = 4, n = 25)$

(c) Degree 7 approximation
$(N = 7, n = 64)$

(d) Degree 8 approximation
$(N = 8, n = 81)$

Figure 1: Shown in each figure is the spherical harmonic approximation of the particle density $\langle f \rangle$ at time $t = 1$, using initial condition (9) and several different values of N. For odd degree approximations, all particles move away from the origin, while for even degree approximations, a substantial amount of particles remain there.

with zero eigenvalue whose first component is nonzero. Because the first component is a multiple of the particle density, this corresponds physically to a nontrivial number of stationary particles. The goal of this paper is to provide a more in-depth analysis of this structure.

Theorem 1. *For N odd, all eigenvectors of $\mathbf{A}_3$ (or $\mathbf{A}_1$, $\mathbf{A}_2$) associated with the eigenvalue 0 have first component equal to zero. For N even, there is an eigenvector of $\mathbf{A}_3$ (or $\mathbf{A}_1$, $\mathbf{A}_2$) associated with the eigenvalue 0 which has first component not equal to zero.*

In the remainder of the paper, we prove Theorem 1 using classical results on spherical harmonics. We also present a few generalizations and related results.

3 Analysis of the eigenstructure

3.1 Preliminaries

Before presenting the main theorems, we prove two lemmas which will form the foundation for the proofs of the main results. The first lemma allows us to use information gained about $\mathbf{A}_3 = \left\langle \Omega_3 \mathbf{Y}\mathbf{Y}^H \right\rangle$ to be used for the matrices $\mathbf{A}_1 = \left\langle \Omega_1 \mathbf{Y}\mathbf{Y}^H \right\rangle$ and $\mathbf{A}_2 = \left\langle \Omega_2 \mathbf{Y}\mathbf{Y}^H \right\rangle$.

Lemma 1. *Given any $\nu, \nu_* \in \mathbb{S}^2$, the matrices $\mathbf{M} := \langle (\nu \cdot \Omega)\mathbf{Y}\mathbf{Y}^H \rangle$ and $\mathbf{M}_* := \langle (\nu_* \cdot \Omega)\mathbf{Y}\mathbf{Y}^H \rangle$ have the same eigenvalues, while their eigenvectors differ by a unitary transformation; that is, if $\mathbf{M}\mathbf{v} = \lambda\mathbf{v}$, then $\mathbf{M}_*(\mathbf{U}\mathbf{v}) = \lambda(\mathbf{U}\mathbf{v})$ for some unitary matrix $\mathbf{U}$. Furthermore, the matrix $\mathbf{U}$ is block diagonal with $\mathbf{U} = diag(\mathbf{U}^{(0)}, \mathbf{U}^{(1)}, \ldots, \mathbf{U}^{(N)})$, where each block $\mathbf{U}^{(\ell)}$ is a square matrix of length $2\ell + 1$.*

Proof. Let Q be an orthogonal matrix such that $\nu_* = Q\nu$. The invariance of the measure $d\Omega$ under orthogonal transformations implies that

$$\mathbf{M}_* = \langle (\nu_* \cdot \Omega)\mathbf{Y}\mathbf{Y}^H \rangle = \langle (\nu \cdot \Omega)\mathbf{P}\mathbf{P}^H \rangle \ , \tag{10}$$

where $\mathbf{P}(\Omega) := \mathbf{Y}(Q\Omega)$. Because the span of the components of $\mathbf{Y}_\ell$ is invariant under orthogonal transformations [5], we can write for each ℓ, $\mathbf{P}_\ell = \mathbf{U}^{(\ell)}\mathbf{Y}_\ell$, where $\mathbf{U}^{(\ell)}$ is a square matrix. Orthonormality of the spherical harmonics implies that $\mathbf{U}^{(\ell)} = \langle \mathbf{P}_\ell \mathbf{Y}_\ell^H \rangle$; thus each $\mathbf{U}^{(\ell)}$ is unitary, since

$$\mathbf{U}^{(\ell)}(\mathbf{U}^{(\ell)})^H = \mathbf{U}^{(\ell)}\langle \mathbf{Y}_\ell \mathbf{P}_\ell^H \rangle = \langle \mathbf{U}^{(\ell)}\mathbf{Y}_\ell \mathbf{P}_\ell^H \rangle = \langle \mathbf{P}_\ell \mathbf{P}_\ell^H \rangle = \mathbf{Id}. \tag{11}$$

Now set $\mathbf{U} = \mathrm{diag}(\mathbf{U}^{(0)}, \mathbf{U}^{(1)}, \ldots \mathbf{U}^{(N)})$. Because $\mathbf{M}$ and $\mathbf{M}_*$ are conjugations of one another, i.e,

$$\mathbf{M}_* = \langle (\nu \cdot \Omega)\mathbf{P}\mathbf{P}^H \rangle = \langle (\nu \cdot \Omega)\mathbf{U}\mathbf{Y}\mathbf{Y}^H\mathbf{U}^H \rangle = \mathbf{U}\mathbf{M}\mathbf{U}^H, \tag{12}$$

their eigenvalues are the same. Furthermore if $\mathbf{M}\mathbf{v} = \lambda\mathbf{v}$, then by (12),

$$\mathbf{M}_*\mathbf{U}\mathbf{v} = \mathbf{U}\mathbf{M}\mathbf{v} = \lambda\mathbf{U}\mathbf{v}. \tag{13}$$

□

The following two properties are a direct consequence of Lemma 1.

Corollary 1. *The matrices $\mathbf{A}_1$, $\mathbf{A}_2$, and $\mathbf{A}_3$ all have the same eigenvalues; moreover, the nonzero eigenvalues come in pairs.*

Proof. It is immediate from the Lemma that $\mathbf{A}_1$, $\mathbf{A}_2$, and $\mathbf{A}_3$ all have the same eigenvalues; one need only choose ν and ν_* to align with any two of the three Cartesian axes. Furthermore, if $\mathbf{A}_i = \langle (\nu \cdot \Omega)\mathbf{Y}\mathbf{Y}^H \rangle$, then $-\mathbf{A}_i = \langle (\nu_* \cdot \Omega)\mathbf{Y}\mathbf{Y}^H \rangle$ with $\nu_* = -\nu$. Hence, A_i and $-A_i$ have the same set of eigenvalues, meaning the nonzero eigenvalues of $\mathbf{A}_i$ must come in pairs. □

Corollary 2. *If $(\lambda, \mathbf{v})$ is an eigenpair of $\mathbf{A}_3$, then there exist unitary matrices $\mathbf{U}_1$ and $\mathbf{U}_2$ such that $(\lambda, \mathbf{U}_1\mathbf{v})$ is an eigenpair of $\mathbf{A}_1$ and $(\lambda, \mathbf{U}_2\mathbf{v})$ is an eigenpair of $\mathbf{A}_2$. Furthermore, because of the block diagonal structures of $\mathbf{U}_1$ and $\mathbf{U}_2$, $v_0^0 = 0$ if and only if $(\mathbf{U}_1\mathbf{v})_0^0 = 0$ if and only if $(\mathbf{U}_2\mathbf{v})_0^0 = 0$.*

As mentioned above, the utility of Lemma 1 is that the study of the eigenstructure in the spherical harmonic equations can be reduced to an analysis of the spectrum of $\mathbf{A}_3$ only. The simplicity of $\mathbf{A}_3$, when compared to $\mathbf{A}_1$ and $\mathbf{A}_2$, is due to the choice of coordinates for expressing the spherical harmonics. Specifically, the form of the third recursion relation in (8) implies that $\mathbf{A}_3$ is diagonal in the k index; that is,

$$[\mathbf{A}_3]_{\ell\ell'}^{kk'} = c_{\ell\ell'}^k \delta^{kk'}\,, \tag{14}$$

where

$$c_{\ell,\ell'}^k = \begin{cases} b_1^k \delta_{1,\ell'}\,, & \ell = 0\,, \\ a_{\ell-1}^k \delta_{\ell-1,\ell'} + b_{\ell+1}^k \delta_{\ell+1,\ell'}\,, & 0 < \ell < N\,, \\ a_{N-1}^k \delta_{N-1,\ell'}\,, & \ell = N\,. \end{cases} \tag{15}$$

Lemma 2. *The eigenvalues of $\mathbf{A}_3$ are the roots of the polynomials $\partial_\mu^{(|j|)} P_{N+1}$ for $|j| \le N$. If λ is a root of $\partial_\mu^{(|j|)} P_{N+1}$, then for any fixed φ, the vector $\mathbf{v}$ with components*

$$v_\ell^k = Y_\ell^j(\cos^{-1}(\lambda), \varphi)\delta^{jk}, \tag{16}$$

is an eigenvector associated with λ.

Remark 1. *The choice of φ in (16) simply introduces a multiplicative constant.*

Proof. Fix j and φ with $|j| \le N$, and let $\partial_\mu^{(|j|)} P_{N+1}(\lambda) = 0$. Then by the definition (4) of the spherical harmonics

$$Y_{N+1}^j(\cos^{-1}(\lambda), \varphi) = 0. \tag{17}$$

From the third recursion relation in (8) and the subsequent decomposition of $\mathbf{A}_3$ in (14),

$$\begin{aligned} \cos\theta Y_\ell^j(\theta,\varphi) &= a_{\ell-1}^j Y_{\ell-1}^j(\theta,\varphi) + b_{\ell+1}^j Y_{\ell+1}^j(\theta,\varphi) \\ &= \sum_{\ell'} [\mathbf{A}_3]_{\ell\ell'}^{jj} Y_{\ell'}^j(\theta,\varphi) + \delta_{\ell N} b_{N+1}^j Y_{N+1}^j(\theta,\varphi). \end{aligned} \tag{18}$$

Setting $\theta = \cos^{-1}(\lambda)$ in (18) gives, using (17),

$$\lambda Y_\ell^j(\cos^{-1}(\lambda),\varphi) = \sum_{\ell'} [\mathbf{A}_3]_{\ell\ell'}^{jj} Y_{\ell'}^j(\cos^{-1}(\lambda),\varphi). \tag{19}$$

Now let $\mathbf{v}$ be given by (16). A direct calculation gives

$$\begin{aligned} (\mathbf{A}_3\mathbf{v})_\ell^k &= \sum_{\ell',k'} [\mathbf{A}_3]_{\ell\ell'}^{kk'} Y_{\ell'}^j(\cos^{-1}(\lambda),\varphi)\delta^{jk'} \\ &= \sum_{\ell'} [\mathbf{A}_3]_{\ell\ell'}^{kk} Y_{\ell'}^j(\cos^{-1}(\lambda),\varphi)\delta^{jk} = \lambda Y_\ell^j(\cos^{-1}(\lambda),\varphi)\delta^{jk} = \lambda v_\ell^k, \end{aligned} \tag{20}$$

which shows that $(\lambda, \mathbf{v})$ is an eigenpair.

We now show that all the eigenvalues are generated in this way by the roots of $\partial_\mu^{(|j|)} P_{N+1}$. From the general properties of Legendre polynomials [1], it is known that $\partial_\mu^{(|j|)} P_{N+1}$ has $N+1-j$ distinct roots. Moreover, it is clear from (16) that the eigenvectors associated to different j are orthogonal. Hence, the roots of $\partial_\mu^{(|j|)} P_{N+1}$, $|j| \le N$, generate distinct eigenvectors. In total there are

$$\sum_{j=-N}^{N} (N+1-|j|) = (2N+1)(N+1) - N(N+1) = (N+1)^2 \tag{21}$$

distinct eigenpairs given by Lemma 2 which, since $\mathbf{A}_3 \colon \mathbb{R}^n \to \mathbb{R}^n$, accounts for all the eigenpairs. $\square$

Remark 2. *Let $\mathbf{A}_3^j$ ($j = -N, \dots, N$) be the diagonal blocks of $\mathbf{A}_3$ with respect to the upper index j:*

$$[\mathbf{A}_3^j]_{\ell\ell'} = [\mathbf{A}_3]_{\ell\ell'}^{jj'} . \tag{22}$$

Then (19) is the eigenvalue problem for $\mathbf{A}_3^j$. Furthermore, if $(\lambda, \mathbf{x})$ is eigenpair of $\mathbf{A}_3^j$, then $(\lambda, \mathbf{v})$, where $v_\ell^k = x_\ell \delta^{jk}$, is an eigenpair of $\mathbf{A}_3$.

Corollary 3. *A basis of the null space of $\mathbf{A}_3$ is given by $\{\mathbf{v}^{(j)} : j = -N, -N+2, \dots, N-2, N\}$, with components*

$$[\mathbf{v}^{(j)}]_\ell^k = Y_\ell^j(\cos^{-1}(0), \varphi)\delta^{jk}. \tag{23}$$

Proof. In Lemma 2, there is an eigenvector corresponding to the eigenvalue $\lambda = 0$ only for indices j such that $\partial_\mu^{(|j|)} P_{N+1}(0) = 0$. This happens if and only if the polynomial is odd which, based on basic properties of Legendre polynomials, happens if and only if $N+1-j$ is odd. Hence a basis is given by vectors of the form (16) with $j = -N, -N+2, \dots, N-2, N$ and $\lambda = 0$. $\square$

3.2 Main results

In this section, we establish Theorem 1 as stated in the introduction as well as other theorems on the null spaces of $\mathbf{A}_1$, $\mathbf{A}_2$, and $\mathbf{A}_3$. All the theorems are specifically stated for $\mathbf{A}_3$, but in light of Lemma 1 and corresponding corollaries, the theorems apply to $\mathbf{A}_1$ and $\mathbf{A}_2$ as well. We restate Theorem 1 for convenience.

Theorem 1. *For N odd, all eigenvectors of $\mathbf{A}_3$ (or $\mathbf{A}_1$, $\mathbf{A}_2$) associated with the eigenvalue 0 have first component equal to zero. For N even, there is an eigenvector of $\mathbf{A}_3$ (or $\mathbf{A}_1$, $\mathbf{A}_2$) associated with the eigenvalue 0 which has first component not equal to zero.*

Proof. Suppose $\mathbf{A}_3\mathbf{v} = 0$. Then $\mathbf{v}$ is a linear combination of basis elements in (23). The $(0,0)$ component of each basis element is

$$[\mathbf{v}^{(j)}]_0^0 = Y_0^0(\cos^{-1}(0), \varphi)\delta^{j,0} , \tag{24}$$

which is nonzero if and only if $j = 0$. According to Corollary 3, the basis does *not* include $\mathbf{v}^{(0)}$, the eigenvector corresponding to the index $j = 0$, when N is odd. Consequently, $[\mathbf{v}]_0^0 = 0$. However, if N is even, then the basis does include $\mathbf{v}^{(0)}$; in particular, $\mathbf{v}^{(0)}$ verifies the second statement of the theorem. $\square$

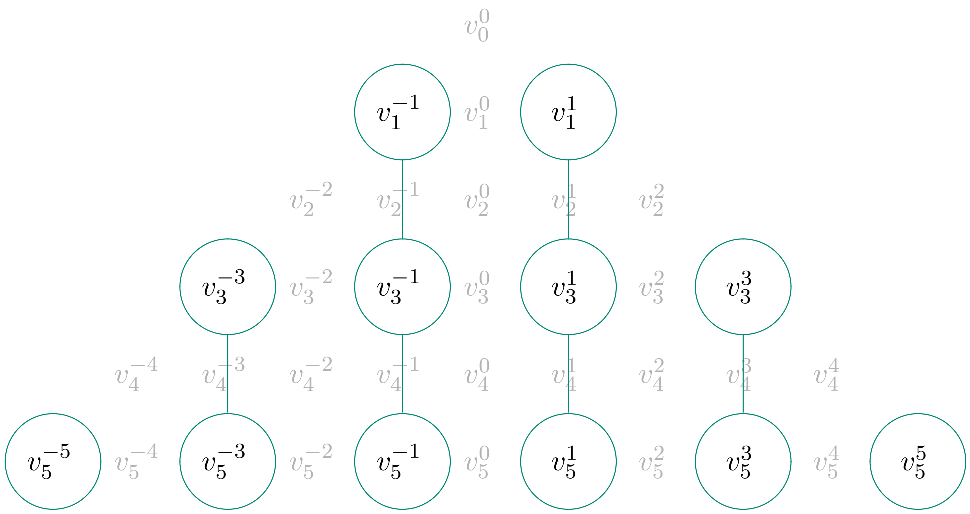


Figure 2: A graphical depiction of $\mathbf{v}$ in the null space of $\mathbf{A}_3$ with $N = 5$ split into rows corresponding to degree ℓ and columns corresponding to order k. Each grayed out entry must be zero. The circled entries indicate possible nonzeros with lines connecting nonzero entries of the basis vectors in (23).

Theorem 2. *The null space of* $\mathbf{A}_3$ *has dimension* $N + 1$.

Proof. The dimension of the null space of $\mathbf{A}_3$ is the number of vectors in the basis (23) which is $N + 1$. $\square$

Theorem 3. *Suppose* $\mathbf{A}_3\mathbf{v} = 0$. *If* N *is odd and either* ℓ *is even or* k *is even, then* $v_\ell^k = 0$. *If* N *is even and either* ℓ *is odd or* k *is odd, then* $v_\ell^k = 0$.

Proof. If N is odd, then the basis in Corollary 3 includes eigenvectors for which j is odd. Thus if k is even (more generally if $k \neq j$), then $[\mathbf{v}^{(j)}]_\ell^k = 0$ for each j. When $k = j$ and ℓ is even, then $\ell - j$ is odd and thus $\partial_\mu^{(|j|)} P_\ell(0) = 0$. This implies $Y_\ell^j(\cos^{-1}(0), \varphi) = 0$ and hence $[\mathbf{v}^j]_\ell^k = 0$. The proof is similar for N even. $\square$

Figure 2 illustrates the conclusion of Theorem 3. The ℓ even cases correspond to the completely grayed out rows and the k even cases correspond to the completely grayed out columns. At least one circled entry in the bottom row ($\ell = N$) must be nonzero. Moreover, the recursion relation in (18) (with $\cos\theta = \lambda = 0$), implies that if one circled entry is nonzero, then so too are all the circled entries in the same column (i.e., with same index k).

Finally, we return to the original motivation of the paper. Recall that for N even, the spherical harmonic method has a qualitative defect which can be interpreted physically as incorrectly predicting a large number of stationary particles in the system. As N increases, it is reasonable to expect that this defect will be suppressed. The next theorem shows this to be the case.

Theorem 4. *If* $\mathbf{v}$ *is in the null space of* $\mathbf{A}_3$ *and* $||\mathbf{v}||_2 = 1$*, then* $v_0^0 \leq \left(\frac{N}{2}+1\right)^{-1/2}$.

Proof. Suppose $\mathbf{A}_3\mathbf{v} = 0$. If N is odd, then by Theorem 1, there is nothing to prove since $v_0^0 = 0$. Suppose then that N is even. Setting $\cos\theta = \lambda = 0$ in (18) yields $a_{\ell-1}^0 v_{\ell-1}^0 + b_{\ell+1}^0 v_{\ell+1}^0 = 0$. Thus because[2] $|b_{\ell+1}^0| < |a_{\ell-1}^0|$, it follows that $|v_0^0| < |v_2^0| < \ldots < |v_{N-2}^0| < |v_N^0|$. Therefore

$$1 \equiv \|\mathbf{v}\|_2^2 \geq \left(v_0^0\right)^2 + \left(v_2^0\right)^2 + \ldots + \left(v_N^0\right)^2 \geq \left(\frac{N}{2}+1\right)\left(v_0^0\right)^2 \,, \tag{25}$$

and this gives the desired result. □

Acknowledgements

This material is based in part upon work supported by the National Science Foundation under Grant No. 1217170.

This research is sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory (ORNL), managed by UT-Battelle, LLC for the U. S. Department of Energy under Contract No. De-AC05-00OR22725.

References

[1] George B Arfken and Hans J Weber. *Mathematical Methods For Physicists International Student Edition.* Academic press, 2005.

[2] T. A. Brunner and J. P. Holloway. Two-dimensional time-dependent Riemann solvers for neutron transport. *J. Comp Phys.*, 210:386–399, 2005.

[3] Thomas A. Brunner. Forms of approximate radiation transport. Technical Report SAND2002-1778, Sandia National Laboratories, 2002.

[4] K. Case and P. Zweifel. *Linear Transport Theory.* Addison-Wesley, Reading, MA, 1967.

[5] Feng Dai and Yuan Xu. *Approximation Theory and Harmonic Analysis on Spheres and Balls.* Springer, New York, 2013.

[6] B. Davison. *Neutron Transport Theory.* Clarendon Press, Oxford, England, 1957.

[7] Herbert Egger and Matthias Schlottbom. A mixed variational framework for the radiative transfer equation. *Mathematical Models and Methods in Applied Sciences*, 22(03), 2012.

[8] Herbert Egger and Matthias Schlottbom. Stationary radiative transfer with vanishing absorption. *Mathematical Models and Methods in Applied Sciences*, 24(05):973–990, 2014.

[9] B. D. Ganapol. Homogeneous infinite media time-dependent analytic benchmarks for X-TM transport methods development. Technical report, Los Alamos National Laboratory, March 1999.

[10] C. Kristopher Garrett and Cory D. Hauck. A comparison of moment closures for linear kinetic transport equations: The line source benchmark. *Transport Theory and Statistical Physics*, 42(6-7):203–235, 2013.

[11] Cory D Hauck and Robert B Lowrie. Temporal regularization of the p_n equations. *Multiscale Modeling & Simulation*, 7(4):1497–1524, 2009.

[12] E. E. Lewis and W. F. Miller, Jr. *Computational Methods of Neutron Transport.* John Wiley and Sons, New York, 1984.

[13] Thomas A Manteuffel, Klaus J Ressel, and Gerhard Starke. A boundary functional for the least-squares finite-element solution of neutron transport problems. *SIAM Journal on Numerical Analysis*, 37(2):556–586, 1999.

[14] G. C. Pomraning. *The Equations of Radiation Hydrodynamics.* Pergamon Press, New York, 1973.

[2] From [2], $a_\ell^0 = \sqrt{\frac{(\ell+1)^2}{(2\ell+3)(2\ell+1)}}$ and $b_\ell^0 = \sqrt{\frac{\ell^2}{(2\ell+1)(2\ell-1)}}$.