Computers and Mathematics with Applications 72 (2016) 264–270

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

On the eigenstructure of spherical harmonic equations for radiative transport

C. Kristopher Garrett[a,*], Cory D. Hauck[a,b]

[a] Computer Science and Mathematics Division, Oak Ridge National Laboratory, USA
[b] Department of Mathematics, University of Tennessee, USA

ARTICLE INFO

Article history:
Available online 24 June 2015

Keywords:
Spherical harmonics
Radiation transport
Odd/even parity
Eigenstructure

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 $\mathbf{u}: \mathbb{R}^3 \times \mathbb{R}^{\geq 0} \to \mathbb{C}^n$ is

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

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 $\sigma_s(x)$ is the scattering cross-section.

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

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

* Corresponding author.
E-mail addresses: garrettck@ornl.gov (C.K. Garrett), hauckc@ornl.gov (C.D. Hauck).

http://dx.doi.org/10.1016/j.camwa.2015.05.030
0898-1221/

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

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

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 $\mathbf{Y}_\ell: \mathbb{S}^2 \to \mathbb{C}^{2\ell+1}$ 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:

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

and $P_\ell: [-1, 1] \to \mathbb{R}$ 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 $\mathbf{Y}: \mathbb{S}^2 \to \mathbb{C}^n$, 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

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

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 [1]:

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

where the nonzero recursion coefficients are known, see [1], 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, [2]. 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 [3, 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 [4, Section 3.5], [3, Appendix D], [5, Section 8.4], [6, Chapter 10], or [7, Section 2.1].) The disadvantages of even N in slab geometry are noted, somewhat in passing, in [4,5,3]. 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 ($\sigma_s = 0$), 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