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Derivation of Spherical Harmonic Approximations to the Nonclassical Particle Transport Equation

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ABSTRACT

The nonclassical transport equation is used to mathematically model transport problems where the particle flux is not exponentially attenuated. In this paper, we apply the spherical harmonics expansion to the nonclassical formulation to derive a system of equations for the nonclassical flux moments. We show that these equations simplify to the well-known classical P_N equations when the free-path distribution function is exponential. Numerical results for test problems in slab-geometry are given to verify the derivation.

KEYWORDS: Nonclassical transport, spherical harmonics, P_N approximations

1. INTRODUCTION

In the past decade, interest in the theory of nonclassical particle transport has increased. This theory focuses on problems in which the distance-to-collision is not exponentially distributed, as is the case in the classical theory of particle transport. Originally motivated by problems arising in measurements of photon path length in the Earth's cloudy atmosphere [1], the nonclassical theory has since provided contributions to transport problems in many other fields, including applications to pebble-bed reactors [2], Lorentz gases [3], and computer graphics [4], to name a few.

The generalized linear Boltzmann equation (GLBE), also known as the nonclassical transport equation, was introduced in [5,6] to address nonclassical transport problems. In this equation the phase space is expanded to include the new independent variable s, a "memory" variable representing the distance traveled by the particle since its previous interaction (the particle's free-path); this was later extended to include angular-dependent free-paths [7]. Different approximations to the GLBE have been proposed, such as nonclassical diffusion [6–8] and nonclassical simplified P_N equations [9,10]. Recently, a deterministic spectral approach was developed, in which the s-dependence is treated through a Laguerre polynomial expansion [11,12]. However, to the best of our knowledge, no attempt has yet been presented to derive spherical harmonic approximations for nonclassical transport, generalizing the P_N approximations to the classical linear Boltzmann equation [13].

In particle transport problems, spherical harmonic (P_N) approximations [14] are often used to eliminate the dependence on the direction-of-flight variable, such that the particle flux is approximated by a truncated Legendre expansion for the angular variable [13]. This paper's main contribution is the derivation of a system of equations for the spherical harmonic moments of the nonclassical particle flux, given in Section 2. In Section 3, we present numerical results for two test problems in slab geometry, comparing the solution of the nonclassical spherical harmonic approximations to those obtained with other established methods, both classical and nonclassical. We conclude this paper with a discussion in Section 4.

2. NONCLASSICAL SPHERICAL HARMONIC APPROXIMATIONS

Let us consider the steady-state, monoenergetic nonclassical linear Boltzmann equation [6]

$$\frac{\partial}{\partial s}\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \boldsymbol{\Omega}\cdot\nabla\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \Sigma_t(s)\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \\ \delta(s)\left[\int_{4\pi}\int_0^{\infty} cP(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\Sigma_t(s')\Psi(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'd\Omega' + Q(\boldsymbol{x},\boldsymbol{\Omega})\right]. \tag{1}$$

Here, $\boldsymbol{x} = (x, y, z)$ is a point in space and $\boldsymbol{\Omega} = (\Omega_x, \Omega_y, \Omega_z) = (\sqrt{1-\mu^2}\cos\omega, \sqrt{1-\mu^2}\sin\omega, \mu)$ is the particle's direction of flight, with ω and μ representing the azimuthal angle and the cosine of the polar angle, respectively. The internal source is represented by $Q(\boldsymbol{x},\boldsymbol{\Omega})$, and s is the distance traveled by the particle since its previous interaction (birth or scattering). Moreover, $\Sigma_t(s)$ is the nonclassical total macroscopic cross section, defined such that $\Sigma_t(s)ds$ represents the probability that a particle, scattered or born at any point $\boldsymbol{x}$ and traveling in the direction $\boldsymbol{\Omega}$, will experience a collision between $\boldsymbol{x} + s\boldsymbol{\Omega}$ and $\boldsymbol{x} + (s + ds)\boldsymbol{\Omega}$. The function $\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)$ denotes the nonclassical particle angular flux, and c represents the scattering ratio, defined as the probability that a particle will scatter after it experiences a collision. The Dirac delta function $\delta(s)$ on the right-hand side of Eq. (1) implies that, when a particle is born or undergoes scattering, its s value is set to 0.

The term $P(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})d\Omega$ denotes the probability that, when a particle with direction of flight $\boldsymbol{\Omega}'$ scatters, its outgoing direction of flight will lie in $d\Omega$ about $\boldsymbol{\Omega}$. We can write $P(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})$ as the Legendre polynomial expansion

$$P(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega}) = \sum_{n'=0}^{\infty}\frac{2n'+1}{4\pi}a_{n'}P_{n'}(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega}), \tag{2}$$

where $P_{n'}(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})$ is the n'-th order Legendre polynomial and $a_{n'}$ is the corresponding expansion coefficient. The Addition Theorem for spherical harmonics [14] states that

$$P_{n'}(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega}) = \frac{4\pi}{2n'+1}\sum_{m'=-n'}^{n'} Y_{n',m'}(\boldsymbol{\Omega})Y^*_{n',m'}(\boldsymbol{\Omega}'), \tag{3}$$

where $Y_{n',m'}$ is the spherical harmonic function of order n' and degree m', defined for $0 \le |m'| \le n'$ by

$$Y_{n',m'}(\boldsymbol{\Omega}) = (-1)^{(m'+|m'|)/2}\left[\frac{2n'+1}{4\pi}\frac{(n'-|m'|)!}{(n'+|m'|)!}\right]^{1/2}(1-\mu^2)^{|m'|/2}\left(\frac{d}{d\mu}\right)^{|m'|}P_{n'}(\mu)e^{im'\omega}, \tag{4}$$

and $Y^*_{n',m'}$ is its complex conjugate, such that $Y_{n',m'}(\boldsymbol{\Omega}) = (-1)^{m'}Y^*_{n',-m'}(\boldsymbol{\Omega})$. Substituting Eqs. (2) and (3) into Eq. (1), we obtain

$$\frac{\partial}{\partial s}\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \boldsymbol{\Omega}\cdot\nabla\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \Sigma_t(s)\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \\ \delta(s)\sum_{n'=0}^{\infty}\sum_{m'=-n'}^{n'} a_{n'}Y_{n',m'}(\boldsymbol{\Omega})\int_0^{\infty}\int_{4\pi} Y^*_{n',m'}(\boldsymbol{\Omega}')c\Sigma_t(s')\Psi(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'd\Omega' + \delta(s)Q(\boldsymbol{x},\boldsymbol{\Omega}). \tag{5}$$

Next, we introduce the following spherical harmonic expansions for the nonclassical angular flux

$$\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\phi_{n,m}(\boldsymbol{x},s)Y_{n,m}(\boldsymbol{\Omega}), \tag{6a}$$

$$\phi_{n,m}(\boldsymbol{x},s) = \int_{4\pi} Y^*_{n,m}(\boldsymbol{\Omega})\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)d\Omega, \tag{6b}$$

and internal source

$$Q(\boldsymbol{x},\boldsymbol{\Omega}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} Q_{n,m}(\boldsymbol{x})Y_{n,m}(\boldsymbol{\Omega})\,, \tag{7a}$$

$$Q_{n,m}(\boldsymbol{x}) = \int_{4\pi} Y^*_{n,m}(\boldsymbol{\Omega})Q(\boldsymbol{x},\boldsymbol{\Omega})d\Omega\,. \tag{7b}$$

With the goal of deriving a system of equations for the nonclassical flux moments defined in Eq. (6b), we substitute Eqs. (6) and (7) into Eq. (5) and then operate on the resulting equation by $\int_{4\pi} Y^*_{n,m}(\boldsymbol{\Omega})(\cdot)d\Omega$. Since the spherical harmonic functions are orthonormal [14], we can use Eqs. (6b) and (7b) to obtain

$$\begin{aligned}
&\frac{\partial}{\partial s}\phi_{n,m}(\boldsymbol{x},s) + \frac{\partial}{\partial x}\int_{4\pi}\Omega_x Y^*_{n,m}(\boldsymbol{\Omega})\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)d\Omega + \\
&\quad\frac{\partial}{\partial y}\int_{4\pi}\Omega_y Y^*_{n,m}(\boldsymbol{\Omega})\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)d\Omega + \frac{\partial}{\partial z}\int_{4\pi}\Omega_z Y^*_{n,m}(\boldsymbol{\Omega})\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)d\Omega + \\
&\qquad\Sigma_t(s)\phi_{n,m}(\boldsymbol{x},s) = \delta(s)\int_0^\infty a_n c\Sigma_t(s')\phi_{n,m}(\boldsymbol{x},s')ds' + \delta(s)Q_{n,m}(\boldsymbol{x}).
\end{aligned} \tag{8}$$

The spherical harmonic functions satisfy [14]

$$\begin{aligned}
\sqrt{1-\mu^2}e^{iw}Y_{n,m}(\boldsymbol{\Omega}) = {}&\left[\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}\right]^{1/2} Y_{n-1,m+1}(\boldsymbol{\Omega}) \\
&- \left[\frac{(n+m+1)(n+m+2)}{(2n+1)(2n+3)}\right]^{1/2} Y_{n+1,m+1}(\boldsymbol{\Omega})\,,
\end{aligned} \tag{9a}$$

$$\begin{aligned}
\sqrt{1-\mu^2}e^{-iw}Y_{n,m}(\boldsymbol{\Omega}) = {}&-\left[\frac{(n+m-1)(n+m)}{(2n-1)(2n+1)}\right]^{1/2} Y_{n-1,m-1}(\boldsymbol{\Omega}) \\
&+ \left[\frac{(n-m+1)(n-m+2)}{(2n+1)(2n+3)}\right]^{1/2} Y_{n+1,m-1}(\boldsymbol{\Omega})\,,
\end{aligned} \tag{9b}$$

$$\mu Y_{n,m}(\boldsymbol{\Omega}) = \left[\frac{n^2-m^2}{(2n-1)(2n+1)}\right]^{1/2} Y_{n-1,m}(\boldsymbol{\Omega}) + \left[\frac{(n+1)^2-m^2}{(2n+1)(2n+3)}\right]^{1/2} Y_{n+1,m}(\boldsymbol{\Omega})\,. \tag{9c}$$

Combining Eqs. (9a) and (9b) yields the useful identities

$$\begin{aligned}
\Omega_x Y_{n,m}(\boldsymbol{\Omega}) &= \sqrt{1-\mu^2}\cos\omega Y_{n,m}(\boldsymbol{\Omega}) = \sqrt{1-\mu^2}\left[\frac{e^{i\omega}+e^{-i\omega}}{2}\right]Y_{n,m}(\boldsymbol{\Omega}) \\
&= \frac{1}{2}\left[\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}\right]^{1/2} Y_{n-1,m+1}(\boldsymbol{\Omega}) \\
&\quad - \frac{1}{2}\left[\frac{(n+m+1)(n+m+2)}{(2n+1)(2n+3)}\right]^{1/2} Y_{n+1,m+1}(\boldsymbol{\Omega}) \\
&\quad - \frac{1}{2}\left[\frac{(n+m-1)(n+m)}{(2n-1)(2n+1)}\right]^{1/2} Y_{n-1,m-1}(\boldsymbol{\Omega}) \\
&\quad + \frac{1}{2}\left[\frac{(n-m+1)(n-m+2)}{(2n+1)(2n+3)}\right]^{1/2} Y_{n+1,m-1}(\boldsymbol{\Omega})\,,
\end{aligned} \tag{10a}$$

$$
\begin{aligned}
\Omega_y Y_{n,m}(\Omega) = \sqrt{1-\mu^2}\sin\omega Y_{n,m}(\mathbf{\Omega}) = \sqrt{1-\mu^2}\left[\frac{e^{i\omega}-e^{-i\omega}}{2i}\right] Y_{n,m}(\mathbf{\Omega}) \\
= -\frac{i}{2}\left[\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}\right]^{1/2} Y_{n-1,m+1}(\mathbf{\Omega}) \\
+ \frac{i}{2}\left[\frac{(n+m+1)(n+m+2)}{(2n+1)(2n+3)}\right]^{1/2} Y_{n+1,m+1}(\mathbf{\Omega}) \\
- \frac{i}{2}\left[\frac{(n+m-1)(n+m)}{(2n-1)(2n+1)}\right]^{1/2} Y_{n-1,m-1}(\mathbf{\Omega}) \\
+ \frac{i}{2}\left[\frac{(n-m+1)(n-m+2)}{(2n+1)(2n+3)}\right]^{1/2} Y_{n+1,m-1}(\mathbf{\Omega})\,.
\end{aligned} \tag{10b}
$$

We use identity (10a) and Eqs. (6) to rewrite the second term in the left-hand side of Eq. (8) as

$$
\begin{aligned}
\frac{\partial}{\partial x}\int_{4\pi}\Omega_x Y^*_{n,m}(\mathbf{\Omega})\Psi(\boldsymbol{x},\mathbf{\Omega},s)d\Omega = \\
\frac{\partial}{\partial x}\Bigg(\frac{1}{2}\left[\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}\right]^{1/2}\phi_{n-1,m+1}(\boldsymbol{x},s) \\
-\frac{1}{2}\left[\frac{(n+m+1)(n+m+2)}{(2n+1)(2n+3)}\right]^{1/2}\phi_{n+1,m+1}(\boldsymbol{x},s) \\
-\frac{1}{2}\left[\frac{(n+m-1)(n+m)}{(2n-1)(2n+1)}\right]^{1/2}\phi_{n-1,m-1}(\boldsymbol{x},s) \\
+\frac{1}{2}\left[\frac{(n-m+1)(n-m+2)}{(2n+1)(2n+3)}\right]^{1/2}\phi_{n+1,m-1}(\boldsymbol{x},s)\Bigg)\,.
\end{aligned} \tag{11a}
$$

Likewise, we use identity (10b) and Eqs. (6) into the third term in the left-hand side of Eq. (8) to obtain

$$
\begin{aligned}
\frac{\partial}{\partial y}\int_{4\pi}\Omega_y Y^*_{n,m}(\mathbf{\Omega})\Psi(\boldsymbol{x},\mathbf{\Omega},s)d\Omega = \\
\frac{\partial}{\partial y}\Bigg(-\frac{i}{2}\left[\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}\right]^{1/2}\phi_{n-1,m+1}(\boldsymbol{x},s) \\
+\frac{i}{2}\left[\frac{(n+m+1)(n+m+2)}{(2n+1)(2n+3)}\right]^{1/2}\phi_{n+1,m+1}(\boldsymbol{x},s) \\
-\frac{i}{2}\left[\frac{(n+m-1)(n+m)}{(2n-1)(2n+1)}\right]^{1/2}\phi_{n-1,m-1}(\boldsymbol{x},s) \\
+\frac{i}{2}\left[\frac{(n-m+1)(n-m+2)}{(2n+1)(2n+3)}\right]^{1/2}\phi_{n+1,m-1}(\boldsymbol{x},s)\Bigg)\,.
\end{aligned} \tag{11b}
$$

Finally, keeping in mind that $\Omega_z = \mu$, we use Eq. (9c) and Eqs. (6) to write the fourth term in the left-hand side of Eq. (8) as

$$
\begin{aligned}
\frac{\partial}{\partial z}\int_{4\pi}\Omega_z Y^*_{n,m}(\mathbf{\Omega})\Psi(\boldsymbol{x},\mathbf{\Omega},s)d\Omega = \\
\frac{\partial}{\partial z}\left(\left[\frac{n^2-m^2}{(2n-1)(2n+1)}\right]^{1/2}\phi_{n-1,m}(\boldsymbol{x},s) + \left[\frac{(n+1)^2-m^2}{(2n+1)(2n+3)}\right]^{1/2}\phi_{n+1,m}(\boldsymbol{x},s)\right)\,.
\end{aligned} \tag{11c}
$$

The results given in Eqs. (11) make it possible to express Eq. (8) in terms of the spherical harmonic moments of the nonclassical angular flux. Equation (8) can now be written as

$$
\begin{aligned}
&\frac{\partial}{\partial s}\phi_{n,m}(\boldsymbol{x},s) \\
&\quad+\frac{\partial}{\partial x}\Bigg(\frac{1}{2}\left[\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}\right]^{1/2}\phi_{n-1,m+1}(\boldsymbol{x},s) \\
&\qquad\qquad-\frac{1}{2}\left[\frac{(n+m+1)(n+m+2)}{(2n+1)(2n+3)}\right]^{1/2}\phi_{n+1,m+1}(\boldsymbol{x},s) \\
&\qquad\qquad\quad-\frac{1}{2}\left[\frac{(n+m-1)(n+m)}{(2n-1)(2n+1)}\right]^{1/2}\phi_{n-1,m-1}(\boldsymbol{x},s) \\
&\qquad\qquad\qquad+\frac{1}{2}\left[\frac{(n-m+1)(n-m+2)}{(2n+1)(2n+3)}\right]^{1/2}\phi_{n+1,m-1}(\boldsymbol{x},s)\Bigg) \\
&\quad+\frac{\partial}{\partial y}\Bigg(-\frac{i}{2}\left[\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}\right]^{1/2}\phi_{n-1,m+1}(\boldsymbol{x},s) \\
&\qquad\qquad+\frac{i}{2}\left[\frac{(n+m+1)(n+m+2)}{(2n+1)(2n+3)}\right]^{1/2}\phi_{n+1,m+1}(\boldsymbol{x},s) \\
&\qquad\qquad\quad-\frac{i}{2}\left[\frac{(n+m-1)(n+m)}{(2n-1)(2n+1)}\right]^{1/2}\phi_{n-1,m-1}(\boldsymbol{x},s) \\
&\qquad\qquad\qquad+\frac{i}{2}\left[\frac{(n-m+1)(n-m+2)}{(2n+1)(2n+3)}\right]^{1/2}\phi_{n+1,m-1}(\boldsymbol{x},s)\Bigg) \\
&\quad+\frac{\partial}{\partial z}\Bigg(\left[\frac{n^2-m^2}{(2n-1)(2n+1)}\right]^{1/2}\phi_{n-1,m}(\boldsymbol{x},s)+\left[\frac{(n+1)^2-m^2}{(2n+1)(2n+3)}\right]^{1/2}\phi_{n+1,m}(\boldsymbol{x},s)\Bigg) \\
&\quad+\Sigma_t(s)\phi_{n,m}(\boldsymbol{x},s)=\delta(s)\int_0^\infty a_n c\Sigma_t(s')\phi_{n,m}(\boldsymbol{x},s')ds'+\delta(s)Q_{n,m}(\boldsymbol{x})\,.
\end{aligned}
\tag{12}
$$

Equation (12) is exactly satisfied by the spherical harmonic expansion coefficients $\phi_{n,m}(\boldsymbol{x},s)$ of the angular flux solution $\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)$ of Eq. (1), for all integers n and m satisfying $0 \leq |m| \leq n$.

The Nonclassical Spherical Harmonic Approximations (NSHA) are attained by selecting positive, odd integer values of N (the order of the approximation) and prescribing the approximation $\phi_{n,m}(\boldsymbol{x},s) = 0$ for all $n > N$. For any given N, the remaining nonzero expansion coefficients are unknowns to be determined, and the resulting approximation to the nonclassical angular flux is:

$$\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) \approx \sum_{n=0}^{N}\sum_{m=-n}^{n}\phi_{n,m}(\boldsymbol{x},s)Y_{n,m}(\boldsymbol{\Omega})\,. \tag{13}$$

If we consider classical transport (i.e., the free-path length distribution being given by an exponential), then Σ_t is independent of s. In that case, we can operate on Eq. (12) by $\int_{-\varepsilon}^{\infty}(\cdot)ds$ to obtain an equation for the classical moments $\phi_{n,m}(\boldsymbol{x}) = \int_0^\infty \phi_{n,m}(\boldsymbol{x},s)ds$. Defining $\phi_{n,m}(\boldsymbol{x},-\varepsilon) = \phi_{n,m}(\boldsymbol{x},\infty) = 0$ takes care of the first term of the equation. Moreover, the product $a_n c\Sigma_t$ is simply the n-th coefficient of the Legendre polynomial expansion for the classical differential scattering cross section [13]

$$\Sigma_s(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') = \sum_{n=0}^{\infty}\frac{2n+1}{4\pi}\left[a_n c\Sigma_t\right]P_n(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') = \sum_{n=0}^{\infty}\frac{2n+1}{4\pi}\left[\Sigma_{s,n}\right]P_n(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')\,. \tag{14}$$

Thus, after operating on Eq. (12) by $\int_{-\varepsilon}^{\infty}(\cdot)ds$, we subtract the first term on the right-hand side from the last term on the left-hand side to obtain $[\Sigma_t - \Sigma_{s,n}]\,\phi_{n,m}$. The resulting equation is the classical first-order partial differential equation for the spherical harmonic moments of the classical angular flux.

3. NUMERICAL RESULTS

In this section we provide a preliminary validation of the proposed method, focusing on obtaining numerical solutions to two test problems in slab-geometry with an isotropic internal source. In this case, Eq. (1) reduces to

$$\frac{\partial}{\partial s}\Psi(z,\mu,s)+\mu\frac{\partial}{\partial z}\Psi(z,\mu,s)+\Sigma_t(s)\Psi(z,\mu,s)= \delta(s)\left[\int_{-1}^{1}\int_0^{\infty} cP(\mu',\mu)\Sigma_t(s')\Psi(z,\mu',s')ds'd\mu'+\frac{Q(z)}{2}\right], \tag{15}$$

and Eq. (12) simplifies to

$$\frac{\partial}{\partial s}\phi_n(z,s)+\frac{\partial}{\partial z}\left(\frac{n}{2n+1}\phi_{n-1}(z,s)+\frac{n+1}{2n+1}\phi_{n+1}(z,s)\right)+\Sigma_t(s)\phi_n(z,s)= \delta(s)\int_0^{\infty} a_n c\Sigma_t(s')\phi_n(z,s')ds'+\delta(s)Q(z)\delta_{n,0}, \tag{16}$$

where $\delta_{n,0}$ is a Kronecker delta.

In this paper we present solutions to the approximations of order $N=1$ and $N=3$. The NSHA of order $N=1$ is given by equations

$$\frac{\partial}{\partial s}\phi_0(z,s)+\frac{\partial}{\partial z}\phi_1(z,s)+\Sigma_t(s)\phi_0(z,s)=\delta(s)\int_0^{\infty} a_0 c\Sigma_t(s')\phi_0(z,s')ds'+Q(z), \tag{17a}$$

$$\frac{\partial}{\partial s}\phi_1(z,s)+\frac{\partial}{\partial z}\left(\frac{1}{3}\phi_0(z,s)\right)+\Sigma_t(s)\phi_1(z,s)=\delta(s)\int_0^{\infty} a_1 c\Sigma_t(s')\phi_1(z,s')ds'; \tag{17b}$$

and the NSHA of order $N=3$ yields the following system:

$$\frac{\partial}{\partial s}\phi_0(z,s)+\frac{\partial}{\partial z}\phi_1(z,s)+\Sigma_t(s)\phi_0(z,s)=\delta(s)\int_0^{\infty} a_0 c\Sigma_t(s')\phi_0(z,s')ds'+\delta(s)Q(z), \tag{18a}$$

$$\frac{\partial}{\partial s}\phi_1(z,s)+\frac{\partial}{\partial z}\left(\frac{1}{3}\phi_0(z,s)+\frac{2}{3}\phi_2(z,s)\right)+\Sigma_t(s)\phi_1(z,s)=\delta(s)\int_0^{\infty} a_1 c\Sigma_t(s')\phi_1(z,s')ds', \tag{18b}$$

$$\frac{\partial}{\partial s}\phi_2(z,s)+\frac{\partial}{\partial z}\left(\frac{2}{5}\phi_1(z,s)+\frac{3}{5}\phi_3(z,s)\right)+\Sigma_t(s)\phi_2(z,s)=\delta(s)\int_0^{\infty} a_2 c\Sigma_t(s')\phi_2(z,s')ds', \tag{18c}$$

$$\frac{\partial}{\partial s}\phi_3(z,s)+\frac{\partial}{\partial z}\left(\frac{3}{7}\phi_2(z,s)\right)+\Sigma_t(s)\phi_3(z,s)=\delta(s)\int_0^{\infty} a_3 c\Sigma_t(s')\phi_3(z,s')ds'. \tag{18d}$$

Equations (17) and (18) were numerically solved using Mark boundary conditions [15] and a similar approach to the one presented in [11,12], i.e., representing the independent variable s in terms of Laguerre polynomials and applying the Diamond Difference method to treat the spatial variable z. We report numerical results for the scalar flux

$$\Phi(z)=\int_{-1}^{1}\int_0^{\infty}\Psi(z,\mu,s)dsd\mu, \tag{19a}$$

where the approximation to the nonclassical angular flux is recovered by the Legendre polynomial expansion

$$\Psi(z,\mu,s)\approx\sum_{n=0}^{N}\frac{2n+1}{2}\phi_n(z,s)P_n(\mu). \tag{19b}$$

As discussed in the previous section, we point out that, for the case of classical transport (Σ_t independent of s), Eq. (15) reduces to the transport equation [6,13]

$$\mu\frac{\partial}{\partial z}\Psi(z,\mu)+\Sigma_t\Psi(z,\mu)=\int_{-1}^{1}\Sigma_s(\mu',\mu)\Psi(z,\mu')d\mu'+\frac{Q(z)}{2}\,, \tag{20}$$

and Eq. (16) reduces to the classical P_N equations in slab geometry

$$\frac{\partial}{\partial z}\left(\frac{n}{2n+1}\phi_{n-1}(z)+\frac{n+1}{2n+1}\phi_{n+1}(z)\right)+\left[\Sigma_t-\Sigma_{s,n}\right]\phi_n(z)=Q(z)\delta_{n,0}\,, \tag{21}$$

with Eqs. (17) and (18) simplifying to their classical P_1 and P_3 counterparts, respectively.

3.1. Test Problem I (Classical Transport)

As a first test, we consider the case of *classical transport* taking place in a 20 cm slab with vacuum boundaries. We assume isotropic scattering, which means $a_0 = 1$ and $a_1 = a_2 = a_3 = 0$ in Eqs. (17) and (18). A spatially uniform source emitting $Q = 1$ particles/cm^{3}s is embedded into the slab.

The slab is centered at the origin ($-10 \leq z \leq 10$) and it is composed of a homogeneous material with total cross section $\Sigma_t(s) = \Sigma_t = 1$ cm^{-1}. In this case, Σ_t is independent of s, and the free-path distribution is simply the exponential $p(s) = e^{-s}$. Under these assumptions, the solution from NSHA should match the one obtained by solving the classical P_N equations.

Table 1 shows the scalar fluxes as defined by Eq. (19a) for three different values of the scattering ratio c at different points in the slab. These were generated by first solving the NSHA in Eqs. (17) and (18) for ϕ_n, and then calculating the nonclassical angular flux according to Eq. (19b). We compared these results with the scalar fluxes obtained by analytically solving the corresponding (classical) P_1 and P_3 equations [16]; the absolute values of the relative differences between these approaches are given in Table 1 as |Relative Deviation|. The results confirm our expectation that the NSHA match the classical P_N approximations when Σ_t is independent of s; in fact, the classical P_1 and P_3 equations are particular cases of the more general Eqs. (17) and (18), respectively.

3.2. Test Problem II (Nonclassical Transport)

For the second test problem, we make only one change in the assumptions of the problem in Section 3.1: we assume the free-path length distribution to be nonexponential, given by the simple gamma distribution [17]

$$p(s) = se^{-s}. \tag{22a}$$

In this case, the nonclassical total cross section is given by

$$\Sigma_t(s) = \frac{s}{1+s}, \tag{22b}$$

and the classical P_N approximations no longer apply.

Table 2 presents the scalar fluxes at different points in the slab for different values of the scattering ratio c, generated with the flux moments obtained by solving Eqs. (17) and (18). To check the accuracy of the NSHA in this problem, we solved Eq. (15) for the nonclassical angular flux $\Psi(z,\mu,s)$ with the method presented in [11], and calculated the scalar flux as in Eq. (19a). These results were compared with the NSHA results, with |Relative Deviation| values also reported in Table 2.

We see that the NSHA yield accurate results for this nonclassical problem. The accuracy of the results improves with increasing N from 1 to 3, and we expect higher values of N to produce more accurate results. Accuracy decreases as one moves further from the center of the slab towards the boundaries, which can be attributed to the Mark boundary conditions used to solve Eqs. (17) and (18) being approximations of the vacuum boundary conditions used in solving Eq. (15).

Table 1: NSHA results and relative deviations from classical P_N solutions

c	Distance $\lvert z\rvert$ from the center of the slab					
	0	2	4	6	8	10
	Scalar flux obtained with NSHA of order $N = 1$ [a]					
0	1.000000 [c]	1.000000	0.999985	0.999516	0.984444	0.500000
0.5	1.999989	1.999935	1.999251	1.991304	1.899064	0.828427
0.9	9.936532	9.894472	9.712544	9.149618	7.459587	2.402467
	$\lvert$Relative deviation$\rvert$ from classical P_1 solution [b]					
0	8.93E-10	1.15E-08	2.75E-07	5.88E-06	9.56E-05	1.00E-17
0.5	5.95E-08	2.79E-07	2.40E-06	1.86E-05	1.13E-04	1.77E-13
0.9	6.08E-06	8.53E-06	1.72E-05	3.55E-05	6.49E-05	5.05E-08
	Scalar flux obtained with NSHA of order $N = 3$ [a]					
0	0.999997	0.999984	0.999837	0.998332	0.982099	0.500000
0.5	1.999933	1.999753	1.998248	1.987304	1.904595	0.828427
0.9	9.930010	9.887637	9.709208	9.178460	7.639344	2.402446
	$\lvert$Relative deviation$\rvert$ from classical P_3 solution [b]					
0	2.84E-08	1.18E-07	8.91E-07	6.21E-06	5.86E-05	5.00E-13
0.5	1.88E-07	5.59E-07	2.96E-06	1.48E-05	8.79E-05	1.87E-11
0.9	5.93E-06	8.06E-06	1.54E-05	3.08E-05	7.08E-05	5.93E-08

a - Scalar flux generated by the solution of Eqs. (17) (for $N = 1$) and Eqs. (18) (for $N = 3$), together with Eqs. (19). The Spectral Approach (SA) [11] was used to deal with the s variable, and the Diamond Difference (DD) method was used to deal with the z variable. The truncation order in the SA is M = 0, and the spatial domain was discretized in 240 nodes in the DD method [12].
b - Scalar flux generated by the analytical solution of the P_1 and P_3 equations [16].
c - Read as 1.000000 particles/cm^{2}s.

4. DISCUSSION

In this study, we have employed spherical harmonics expansions to the nonclassical transport equation to derive nonclassical spherical harmonic approximations (NSHA). In the general case described in Eq. (12), an approximation of degree N contains $(N+1)^2$ expansion coefficients $\phi_{n,m}(\boldsymbol{x}, s)$ and $(N+1)^2$ equations. We have shown that, if we consider the total cross section to be independent of the free-path s, the nonclassical spherical harmonic equation (12) simplifies to its well-known classical P_N counterpart.

We have presented numerical results for two test problems in slab geometry, confirming that (i) the P_N approximations are a particular case of the NSHA, being equivalent in the case of classical transport; and (ii) the NSHA can be used to approximate solutions of the nonclassical transport equation for nonexponential free-path distributions.

It is important to point out that Eqs. (12) and (16) (and, consequently, Eqs. (17) and (18)) are integro-differential equations for the flux moments, with an improper integral in the free-path variable s. These are significantly more complex than the first-order partial differential equations for the flux moments in the classical P_N approximation, which means that current P_N codes cannot be used to directly solve these nonclassical equations. It also means that one cannot easily eliminate the odd-order spherical harmonic flux moments, which can be done in classical P_N equations to obtain a system of coupled second-order partial differential equations for the even-order flux moments.

In future work, we will attempt to establish a connection between the NSHA and the previously derived

Table 2: NSHA results and relative deviations from nonclassical transport solutions

c	Distance $\lvert z\rvert$ from the center of the slab					
	0	2	4	6	8	10
	Scalar flux obtained with NSHA of order $N = 1$ [a]					
0	1.999999 [c]	1.999993	1.999813	1.995661	1.914716	1.000000
0.5	3.998388	3.995758	3.979284	3.895212	3.470627	1.595865
0.9	18.746047	18.474119	17.540398	15.539919	11.605984	4.370842
	$\lvert$Relative deviation$\rvert$ from nonclassical transport solution [b]					
0	2.43E-05	9.03E-05	6.06E-04	3.23E-03	6.01E-04	1.10E-09
0.5	4.05E-04	7.01E-04	1.70E-03	2.15E-03	1.60E-02	6.70E-03
0.9	6.62E-04	1.49E-03	4.83E-03	1.44E-02	4.43E-02	1.10E-02
	Scalar flux obtained with NSHA of order $N = 3$ [a]					
0	1.999957	1.999817	1.998536	1.988883	1.919310	1.000000
0.5	3.996753	3.992885	3.972122	3.886158	3.533263	1.600203
0.9	18.750404	18.492001	17.610049	15.741791	12.106256	4.391332
	$\lvert$Relative deviation$\rvert$ from nonclassical transport solution [b]					
0	3.35E-06	2.65E-06	3.27E-05	1.81E-04	3.00E-03	1.10E-09
0.5	3.75E-06	1.83E-05	9.95E-05	1.80E-04	1.80E-03	4.00E-03
0.9	4.30E-04	5.28E-04	8.75E-04	1.57E-03	3.11E-03	6.34E-03

a - Scalar flux generated by the solution of Eqs. (17) (for $N = 1$) and Eqs. (18) (for $N = 3$), together with Eqs. (19). The Spectral Approach (SA) [11] was used to deal with the s variable, and the Diamond Difference (DD) method was used to deal with the z variable. The truncation order in the SA is M = 2, and the spatial domain was discretized in 240 nodes in the DD method [12].
b - Scalar flux generated by solving Eq. (15) with the procedure presented in [11].
c - Read as 1.999999 particles/cm^{2}s.

nonclassical Simplified P_N (nonclassical SP_N) equations [9,10]. These equations only contain the *moments* of the free-path distribution as input parameters, with s not being present as an independent variable, which makes them compatible with current SP_N codes. We will also explore problems with different free-path distributions, and will work on numerical solutions for problems with anisotropic scattering and higher spatial dimensions. In addition, we will investigate how different choices of boundary conditions [18] affect the solutions of the NSHA for different problems.

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