

CONF-950420--6

LA-UR 94-3380

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

TITLE: **ASYMPTOTIC DERIVATION OF THE MULTIGROUP  $P_1$  AND SIMPLIFIED  $P_N$  EQUATIONS WITH ANISOTROPIC SCATTERING**

AUTHOR(S): Edward W. Larsen  
J.E. Morel, CIC-3  
John M. McGhee, CIC-3

SUBMITTED TO: International Conference on Mathematics and Computations Reactor Physics,  
and Environmental Analyses  
Portland, Oregon  
April 30-May 4, 1995

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Los Alamos National Laboratory  
Los Alamos New Mexico 87545

# ASYMPTOTIC DERIVATION OF THE MULTIGROUP $P_1$ AND SIMPLIFIED $P_N$ EQUATIONS WITH ANISOTROPIC SCATTERING

Edward W. Larsen  
Department of Nuclear Engineering  
University of Michigan  
Ann Arbor, Michigan 48109  
(313) 936-0124

J.E. Morel and John M. McGhee  
Los Alamos National Laboratory  
P.O. Box 1663, MS-B265  
Los Alamos, New Mexico 87545  
(505) 667-6091

## ABSTRACT

The multigroup  $P_1$  and Simplified  $P_N$  equations are shown to be a family of asymptotic approximation to the multigroup transport equation with anisotropic scattering. The physical assumptions are that the material system is optically thick, the probability of absorption is small, and the mean scattering angle  $\bar{\mu}_0$  is not close to unity.

## I. INTRODUCTION

The Simplified  $P_N$  ( $SP_N$ ) equations were originally proposed by Gelbard in the early 1960's as a relatively easy way to include additional transport physics into the  $P_1$  model without resorting to the more complicated  $P_N$  equations.<sup>1-3</sup> During the succeeding 30 years, other researchers<sup>4-13</sup> have experimented computationally with the  $SP_N$  equations and have usually concluded that  $SP_N$  solutions are significantly more transport-like than diffusion solutions. For example, Gamino<sup>12,13</sup> has reported that low-order  $SP_N$  solutions often capture "greater than 80%" of the transport corrections to diffusion theory.

One of the reasons for this success is that in planar geometry, the  $SP_N$  equations exactly reduce to the  $P_N$  (and hence  $S_{N+1}$ ) equations. However, recent theoretical work<sup>14-21</sup> has explained other reasons for these successful computational results:  $SP_N$  theory is an asymptotic correction to  $P_1$  theory for problems in which  $P_1$  theory is an asymptotic approximation to transport theory. Also, the  $SP_N$  equations have been derived variationally in certain cases. These asymptotic and variational derivations have mostly been limited to one-group transport problems with isotropic scattering. However, Larsen has recently sketched a derivation of the  $SP_N$  equations for multigroup transport problems with isotropic scattering.<sup>19</sup>

In this paper, we extend the analysis in Ref. 19 and derive the  $SP_N$  equations as an asymptotic limit of the fully general 3-D multigroup transport equation with arbitrary anisotropic scattering. Our physical assumptions are that the system is optically thick, that scattering dominates absorption, and that the mean scattering angle  $\bar{\mu}_0$  is not close to unity. In such circumstances, we show that multigroup  $P_1$  theory is the leading-order asymptotic expansion of the transport equation, that multigroup  $SP_2$  theory is the first asymptotic correction to  $P_1$  theory, and that multigroup  $SP_3$  theory is the second asymptotic correction to  $P_1$  theory. Our analysis can be continued for  $N > 3$ , but we will not do so here.

The remainder of this paper is organized as follows. In Sec. II we establish notation and derive, by the conventional method, the multigroup  $SP_2$  and  $SP_3$  equations. In Sec. III we asymptotically derive the multigroup  $P_1$ ,  $SP_2$ , and  $SP_3$  equations. We conclude with numerical results in Sec. IV and a brief discussion in Sec. V.

## II. CONVENTIONAL DERIVATION OF THE $SP_N$ EQUATIONS

We shall consider the multigroup transport equation

$$\Omega_i \frac{\partial}{\partial x_i} \psi(\mathbf{x}, \Omega) + \Sigma_t(\mathbf{x}) \psi(\mathbf{x}, \Omega) = \int_{4\pi} \Sigma_s(\mathbf{x}, \Omega \cdot \Omega') \psi(\mathbf{x}, \Omega') d^2 \Omega' + \frac{Q(\mathbf{x})}{4\pi}, \quad \mathbf{x} \in V, \quad |\Omega| = 1, \quad (1)$$

defined in a physical region  $V$ . The notation in Eq. (1) is standard:  $\underline{x} = (x_1, x_2, x_3)$  is the spatial variable;  $\underline{\Omega} = (\Omega_1, \Omega_2, \Omega_3)$  with  $|\underline{\Omega}| = 1$  is the angular variable;  $\psi(\underline{x}, \underline{\Omega})$  is a  $G \times 1$  vector whose  $g$ -th component is the angular flux of neutrons in group  $g$  at the point  $\underline{x}$  travelling in the direction  $\underline{\Omega}$ ;  $\Sigma_t(\underline{x})$  is the total cross section (a  $G \times G$  diagonal matrix),  $\Sigma_s(\underline{x}, \mu_0)$  is the differential scattering cross section (a  $G \times G$  matrix);  $Q(\underline{x})$  is the interior source (a  $G \times 1$ ) vector; and we use the summation convention: repeated subscripts are summed from 1 to 3. The boundary condition is

$$\psi(\underline{x}, \underline{\Omega}) = \psi^b(\underline{x}, \underline{\Omega}) \quad , \quad \underline{x} \in \partial V \quad , \quad \underline{\Omega} \cdot \underline{n} < 0 \quad , \quad (2)$$

where  $\psi^b$  is the prescribed incident angular flux and  $\underline{n}$  is the unit outer normal. The differential scattering cross section has the expansion

$$\Sigma_s(\underline{x}, \mu_0) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} \Sigma_{s,n}(\underline{x}) P_n(\mu_0) \quad , \quad (3)$$

where  $P_n(\mu)$  is the Legendre polynomial of order  $n$ .

The standard derivation of the  $SP_N$  equations is partly motivated by the following observation. If we write the planar-geometry  $P_1$  equations that correspond to Eq. (1),

$$\frac{d}{dx} \phi_1(x) + [\Sigma_t(x) - \Sigma_{s0}(x)] \phi_0(x) = Q(x) \quad , \quad (4)$$

$$\frac{1}{3} \frac{d}{dx} \phi_1(x) + [\Sigma_t(x) - \Sigma_{s1}(x)] \phi_1(x) = 0 \quad , \quad (5)$$

and we formally

1. replace the scalar derivative  $\frac{d}{dx}$  by the gradient operator  $\frac{\partial}{\partial x_i}$ ,
2. replace all odd-order moments  $\phi_n(x)$  by  $\phi_{n,i}(\underline{x})$ ,
3. replace all even-order moments  $\phi_n(x)$  by  $\phi_n(\underline{x})$ ,

then we obtain

$$\frac{\partial}{\partial x_i} \phi_{1,i}(\underline{x}) + [\Sigma_t(\underline{x}) - \Sigma_{s0}(\underline{x})] \phi_0(\underline{x}) = Q(\underline{x}) \quad , \quad (6)$$

$$\frac{1}{3} \frac{\partial}{\partial x_i} \phi_0(\underline{x}) + [\Sigma_t(\underline{x}) - \Sigma_{s1}(\underline{x})] \phi_{1,i}(\underline{x}) = 0 \quad , \quad i = 1, 2, 3 \quad . \quad (7)$$

These are the familiar 3-D multigroup  $P_1$  equations. By using Eq. (7) to eliminate  $\phi_{1,i}$  from Eq. (6), we obtain the following system of  $G$  coupled diffusion equations in the  $G$  unknowns  $\phi_0(\underline{x})$ :

$$-\frac{\partial}{\partial x_i} \left( \frac{1}{3} \Sigma_{s1}^{-1} \right) \frac{\partial}{\partial x_i} \phi_0 + \Sigma_{a0} \phi_0 = Q \quad . \quad (8)$$

(Here we have defined the  $G \times G$  matrices

$$\Sigma_{an} \equiv \Sigma_t - \Sigma_{s,n} \quad , \quad n \geq 0 \quad .) \quad (9)$$

Also, boundary conditions for Eqs. (6) and (7) [or (8)] can be obtained formally from planar-geometry boundary conditions for Eqs. (4) and (5) by simply replacing  $\phi_1$  by  $n_i \phi_{1,i}$  (where, again,  $\underline{n} = (n_1, n_2, n_3)$  is the unit outer normal).

Applying this same formal procedure to the planar-geometry  $P_2$  equations, one obtains the following  $SP_2$  equations:

$$\frac{\partial}{\partial x_i} \phi_{1,i}(\underline{x}) + \Sigma_{a0}(\underline{x}) \phi_0(\underline{x}) = Q(\underline{x}) \quad , \quad (10)$$

$$\frac{\partial}{\partial x_i} \left[ \frac{1}{3} \phi_0(\underline{x}) + \frac{2}{3} \phi_2(\underline{x}) \right] + \Sigma_{a1}(\underline{x}) \phi_{1,i}(\underline{x}) = 0 \quad , \quad i = 1, 2, 3 \quad , \quad (11)$$

$$\frac{\partial}{\partial \mathbf{x}_i} \left[ \frac{2}{5} \phi_{1,i}(\mathbf{x}) \right] + \Sigma_{a2}(\mathbf{x}) \phi_2(\mathbf{x}) = 0 \quad . \quad (12)$$

By using Eqs. (11) and (12) to eliminate  $\phi_{1,i}$  and  $\phi_2$  from Eqs. (10), one reduces these equations to the following G coupled diffusion equations in the G unknowns  $\phi_i(\mathbf{x})$ :

$$-\frac{\partial}{\partial \mathbf{x}_i} \left( \frac{1}{3} \Sigma_{a1}^{-1} \right) \frac{\partial}{\partial \mathbf{x}_i} \left[ \phi_0 + \frac{4}{5} \Sigma_{a2}^{-1} (\Sigma_{a0} \phi_0 - Q) \right] + \Sigma_{a0} \phi_0 = Q \quad . \quad (13)$$

In contrast, the full  $P_2$  equations have 9G equations and unknowns. Boundary conditions for Eqs. (10)-(12) [or (13)] can be obtained from planar-geometry conditions using the same formal procedure as with the  $P_1$  equations.

Also, applying the same formal procedure to the planar geometry  $P_3$  equations, one obtains the following  $SP_3$  equations:

$$\frac{\partial}{\partial \mathbf{x}_i} \phi_{1,i}(\mathbf{x}) + \Sigma_{a0}(\mathbf{x}) \phi_0(\mathbf{x}) = Q(\mathbf{x}) \quad , \quad (14)$$

$$\frac{\partial}{\partial \mathbf{x}_i} \left[ \frac{1}{3} \phi_0(\mathbf{x}) + \frac{2}{3} \phi_2(\mathbf{x}) \right] + \Sigma_{a1}(\mathbf{x}) \phi_{1,i}(\mathbf{x}) = 0 \quad , \quad i = 1, 2, 3 \quad , \quad (15)$$

$$\frac{\partial}{\partial \mathbf{x}_i} \left[ \frac{2}{5} \phi_{1,i}(\mathbf{x}) + \frac{3}{5} \phi_{3,i}(\mathbf{x}) \right] + \Sigma_{a2}(\mathbf{x}) \phi_2(\mathbf{x}) = 0 \quad , \quad (16)$$

$$\frac{\partial}{\partial \mathbf{x}_i} \left[ \frac{3}{7} \phi_2(\mathbf{x}) \right] + \Sigma_{a3}(\mathbf{x}) \phi_{3,i}(\mathbf{x}) = 0 \quad , \quad i = 1, 2, 3 \quad . \quad (17)$$

By using Eqs. (15) and (17) to eliminate  $\phi_{1,i}$  and  $\phi_{3,i}$  from Eqs. (14) and (16), and slightly rearranging, one obtains the following 2G coupled diffusion equations in the 2G unknowns  $\phi_0(\mathbf{x})$  and  $\phi_2(\mathbf{x})$ :

$$-\frac{\partial}{\partial \mathbf{x}_i} \left( \frac{1}{3} \Sigma_{a1}^{-1} \right) \frac{\partial}{\partial \mathbf{x}_i} (\phi_0 + 2\phi_2) + \Sigma_{a0} \phi_0 = Q \quad , \quad (18)$$

$$-\frac{\partial}{\partial \mathbf{x}_i} \left( \frac{9}{35} \Sigma_{a3}^{-1} \right) \frac{\partial}{\partial \mathbf{x}_i} \phi_2 + \Sigma_{a2} \phi_2 = \frac{2}{5} (\Sigma_{a0} \phi_0 - Q) \quad . \quad (19)$$

In contrast, the full  $P_3$  equations have 16G equations and unknowns. Boundary conditions for Eqs. (14)-(17) can be obtained from planar-geometry conditions using the same formal procedure as with the  $P_1$  equations.

Of course, the above derivations of the  $SP_2$  and  $SP_3$  equations are ad-hoc. This apparant lack of a solid theoretical basis has likely contributed to the historical neglect of the  $SP_N$  equations, even though the computational experience with these equations has been quite favorable.

### III. ASYMPTOTIC DERIVATION OF THE $P_1$ AND $SP_N$ EQUATIONS

We consider Eq. (1) for optically thick systems that are dominated by scattering, for which scattering is not extremely forward-peaked, and for which the solution  $\psi$  is  $O(1)$ . Such a situation occurs if  $\Sigma_t$ ,  $\Sigma_s$ , and  $Q$  satisfy:

$$\Sigma_t(\mathbf{x}) = \frac{1}{\epsilon} \sigma_t(\mathbf{x}) \quad , \quad (20)$$

$$\Sigma_{sn}(\mathbf{x}) = \frac{1}{\epsilon} \sigma_{sn}(\mathbf{x}) \quad , \quad n \geq 0 \quad , \quad (21)$$

$$Q(\mathbf{x}) = \epsilon q(\mathbf{x}) \quad , \quad (22)$$

$$\sup_{\|u\|=1} \|(\sigma_t - \sigma_{sn})^{-1} u\| = \begin{cases} O(\epsilon^{-2}) & , \quad n = 0 \\ O(1) & , \quad n \geq 1 \end{cases} \quad , \quad (23)$$

where  $\sigma_t$ ,  $\sigma_s$ , and  $q$  are  $O(1)$  and  $\epsilon$  is a small, positive dimensionless parameter. Eq. (20) implies that the mean free path is small, of  $O(\epsilon)$ , so the system  $V$  is  $O(\epsilon^{-1})$  mean free paths thick. It can be shown that Eq. (23) for  $n = 0$

holds if the probability of absorption is small, of  $O(\epsilon^2)$ , and for  $n \geq 1$  holds if scattering is not highly forward-peaked. (These results are independent of the kind of group-to-group coupling that exists due to scattering; these coupling terms can be  $O(1)$ , or they can be small.) Eqs. (20)-(23) imply that the infinite-medium solution

$$\psi = \frac{1}{4\pi} (\Sigma_t - \Sigma_{s0})^{-1} Q = \frac{1}{4\pi} \left[ \frac{1}{\epsilon} (\sigma_t - \sigma_{s0}) \right]^{-1} \epsilon q = \frac{1}{4\pi} (\sigma_t - \sigma_{s0})^{-1} \epsilon^2 q \quad (24)$$

is  $O(1)$ . If we define

$$\sigma_s(\underline{x}, \mu_0) = \epsilon \Sigma_s(\underline{x}, \mu_0) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} \sigma_{s,n}(\underline{x}) P_n(\mu_0) \quad , \quad (25)$$

then Eq. (1) may be written as

$$\Omega_i \frac{\partial}{\partial x_i} \psi(\underline{x}, \underline{\Omega}) + \frac{1}{\epsilon} \sigma_t(\underline{x}) \psi(\underline{x}, \underline{\Omega}) = \frac{1}{\epsilon} \int_{4\pi} \sigma_s(\underline{x}, \underline{\Omega} \cdot \underline{\Omega}') \psi(\underline{x}, \underline{\Omega}') d^2 \Omega' + \epsilon \frac{q(\underline{x})}{4\pi} \quad (26)$$

Now, let us define

$$\phi_0(\underline{x}) = \int_{4\pi} \psi(\underline{x}, \underline{\Omega}') d^2 \Omega' \quad , \quad (27)$$

$$\phi_1(\underline{x}) = \int_{4\pi} \underline{\Omega}' \psi(\underline{x}, \underline{\Omega}') d^2 \Omega' \quad , \quad (28)$$

$$P\psi(\underline{x}, \underline{\Omega}) = \frac{1}{4\pi} \int_{4\pi} \psi(\underline{x}, \underline{\Omega}') d^2 \Omega' \quad . \quad (29)$$

Operating on Eq. (26) by  $P$  and  $(I - P)$ , we obtain the balance equation

$$\frac{\partial}{\partial x_i} \phi_{1,i} + \frac{1}{\epsilon} (\sigma_t - \sigma_{s0}) \phi_0 = \epsilon q \quad , \quad (30)$$

and

$$(I - P) \Omega_i \frac{\partial}{\partial x_i} \psi + \frac{\sigma_t}{\epsilon} \left( \psi - \frac{1}{4\pi} \phi_0 \right) = \frac{1}{\epsilon} \int_{4\pi} \left( \sum_{n=1}^{\infty} \frac{2n+1}{4\pi} \sigma_{s,n} P_n(\underline{\Omega} \cdot \underline{\Omega}') \right) \psi(\underline{x}, \underline{\Omega}') d^2 \Omega' \quad (31)$$

If we define the operator  $L$  by

$$L\psi(\underline{x}, \underline{\Omega}) \equiv \sigma_t \psi(\underline{x}, \underline{\Omega}) - \int_{4\pi} \left( \sum_{n=1}^{\infty} \frac{2n+1}{4\pi} \sigma_{s,n} P_n(\underline{\Omega} \cdot \underline{\Omega}') \right) \psi(\underline{x}, \underline{\Omega}') d^2 \Omega' \quad , \quad (32)$$

then Eq. (31) may be written more compactly as

$$L\psi + \epsilon (I - P) \Omega_i \frac{\partial}{\partial x_i} \psi = \frac{\sigma_t}{4\pi} \phi_0 \quad . \quad (33)$$

$L$  is very similar to the collision operator [the  $O(\epsilon^{-1})$ ] terms in Eq. (26), but  $L$  does not contain the  $n = 0$  part of the scattering operator. Thus, if scattering is isotropic,  $L$  reduces to a simple multiplicative operator. Also, from the assumptions (23),  $L^{-1}$  exists and is  $O(1)$ . Thus, Eq. (33) may be written

$$\left[ I + \epsilon L^{-1} (I - P) \Omega_i \frac{\partial}{\partial x_i} \right] \psi = \frac{1}{4\pi} \phi_0 \quad . \quad (34)$$

Hence,

$$\psi = \left[ I + \epsilon L^{-1} (I - P) \Omega_i \frac{\partial}{\partial x_i} \right]^{-1} \frac{\phi_0}{4\pi} \quad , \quad (35)$$

and introducing this into Eq. (28), we obtain

$$\phi_{1,i}(\underline{x}) = \frac{1}{4\pi} \int_{4\pi} \Omega_i \left[ I + \epsilon L^{-1} (I - P) \Omega_j \frac{\partial}{\partial x_j} \right]^{-1} \phi_0(\underline{x}) d^2 \Omega \quad . \quad (36)$$

Eqs. (30) and (36) are an exact system of equations for the scalar flux  $\phi_0$  and the current  $\phi_{1,i}$ . However, Eq. (36) is too complicated to be of immediate use, so we shall approximate it by expanding it for  $\varepsilon \ll 1$ . The result is:

$$\phi_{1,i}(\underline{x}) \approx \sum_{n=0}^{\infty} \varepsilon^n L_{i,n} \phi(\underline{x}) \quad , \quad (37)$$

where the operators  $L_{i,n}$  are defined by:

$$L_{i,n} \phi(\underline{x}) = \frac{(-1)^n}{4\pi} \int_{4\pi} \Omega_i [L^{-1}(I - P)\Omega \cdot \nabla]^n \phi_0(\underline{x}) d^2\Omega \quad . \quad (38)$$

The first few operators  $L_{i,n}$  can easily be evaluated using the following facts, which we state without proof.

1. For each  $i$ , the quantity

$$\omega_i \equiv \Omega_i \quad (39)$$

is a linear combination of spherical harmonic functions of order 1.

2. For each  $i$  and  $j$ , the quantity

$$\omega_{i,j} \equiv \Omega_i \Omega_j - \frac{1}{3} \delta_{i,j} \quad (40)$$

is a linear combination of spherical harmonic functions of order 2.

3. For each  $i, j$ , and  $k$ , the quantity

$$\omega_{i,j,k} \equiv \Omega_i \Omega_j \Omega_k - \frac{1}{5} (\Omega_i \delta_{j,k} + \Omega_j \delta_{k,i} + \Omega_k \delta_{i,j}) \quad (41)$$

is a linear combination of spherical harmonic functions of order 3.

4. For each  $i, j, k$ , and  $l$ , the quantity

$$\begin{aligned} \omega_{i,j,k,l} \equiv & \Omega_i \Omega_j \Omega_k \Omega_l - \frac{1}{7} (\Omega_i \Omega_j \delta_{k,l} + \Omega_i \Omega_k \delta_{j,l} + \Omega_i \Omega_l \delta_{j,k} + \Omega_j \Omega_k \delta_{i,l} + \Omega_j \Omega_l \delta_{i,k} + \Omega_k \Omega_l \delta_{i,j}) \\ & + \frac{1}{35} (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \end{aligned} \quad (42)$$

is a linear combination of spherical harmonic functions of order 4.

Therefore, with  $L$  defined by Eq. (32), one has

$$L^{-1} \omega_i = (\sigma_1 - \sigma_{s1})^{-1} \omega_i \quad , \quad (43)$$

$$L^{-1} \omega_{ij} = (\sigma_1 - \sigma_{s2})^{-1} \omega_{ij} \quad , \quad (44)$$

$$L^{-1} \omega_{ijk} = (\sigma_1 - \sigma_{s3})^{-1} \omega_{ijk} \quad , \quad (45)$$

$$L^{-1} \omega_{ijkl} = (\sigma_1 - \sigma_{s3})^{-1} \omega_{ijkl} \quad . \quad (46)$$

We will now explicitly calculate  $L_{i,0}$  and  $L_{i,1}$ . For  $n = 0$ ,

$$L_{i,0} \phi = \frac{1}{4\pi} \int_{4\pi} \Omega_i \phi d^2\Omega = \left( \frac{1}{4\pi} \int_{4\pi} \Omega_i d^2\Omega \right) \phi = 0 \quad , \quad (47)$$

because the integrand is an odd function of  $\Omega$ . For  $n = 1$ ,

$$L^{-1}(I - P)\Omega \cdot \nabla \phi = L^{-1} \omega_j \frac{\partial}{\partial x_j} \phi = (\sigma_1 - \sigma_{s1})^{-1} \omega_j \frac{\partial}{\partial x_j} \phi = (\sigma_1 - \sigma_{s1})^{-1} \Omega_j \frac{\partial}{\partial x_j} \phi \quad . \quad (48)$$

Therefore, if we define

$$\sigma_{an} = \sigma_t - \sigma_{,n} = \varepsilon \Sigma_{an} \quad , \quad n \geq 0 \quad , \quad (49)$$

then, using Eq. (40)

$$\begin{aligned} L_{i,1}\phi &= -\frac{1}{4\pi} \int_{4\pi} \Omega_i \sigma_{a1}^{-1} \Omega_j \frac{\partial}{\partial x_j} \phi d^2\Omega = -\left(\frac{1}{4\pi} \int_{4\pi} \Omega_i \Omega_j d^2\Omega\right) \sigma_{a1}^{-1} \frac{\partial}{\partial x_j} \phi \\ &= -\left[\frac{1}{4\pi} \int_{4\pi} \left(\omega_{ij} + \frac{1}{3} \delta_{ij}\right) d^2\Omega\right] \sigma_{a1}^{-1} \frac{\partial}{\partial x_j} \phi = -\frac{1}{3} \delta_{ij} \sigma_{a1}^{-1} \frac{\partial}{\partial x_j} \phi = -\frac{1}{3} \sigma_{a1}^{-1} \frac{\partial}{\partial x_i} \phi \quad . \end{aligned} \quad (50)$$

Proceeding in this manner, using Eqs. (39)-(46), we obtain

$$L_{i,n}\phi = 0 \quad \text{for } n \text{ even} \quad , \quad (51)$$

because for  $n$  even, the integral defining  $L_{i,n}$  has an integrand which is an odd function of  $\underline{\Omega}$ . For  $n$  odd, the operators  $L_{i,n}$  do not vanish and are quite complicated. However, for homogeneous-medium problems, or for heterogeneous-medium problems in which the solution behaves nearly one-dimensionally near interfaces (i.e. tangential directional derivatives at interfaces can be ignored), these operators simplify. If for  $n \geq 1$  we define

$$M_n \equiv \frac{\partial}{\partial x_j} \sigma_{an}^{-1} \frac{\partial}{\partial x_j} \equiv \nabla \cdot \sigma_{an}^{-1} \nabla \quad , \quad (52)$$

then we obtain

$$L_{i,3}\phi = -\sigma_{a1}^{-1} \frac{\partial}{\partial x_i} \sigma_{a2}^{-1} \left(\frac{4}{45} M_1\right) \phi \quad , \quad (53)$$

and

$$L_{i,5}\phi = -\sigma_{a1}^{-1} \frac{\partial}{\partial x_i} \sigma_{a2}^{-1} \left(\frac{16}{675} M_1 + \frac{4}{175} M_3\right) \sigma_{a2}^{-1} M_1 \phi \quad . \quad (54)$$

Thus, Eqs. (37) and (50)-(54) give

$$\phi_{1,i} = -\varepsilon \sigma_{a1}^{-1} \frac{\partial}{\partial x_i} \left[\frac{1}{3} \phi + \varepsilon^2 \sigma_{a2}^{-1} \left(\frac{4}{45} M_1\right) \phi + \varepsilon^4 \sigma_{a2}^{-1} \left(\frac{16}{675} M_1 + \frac{4}{175} M_3\right) \sigma_{a2}^{-1} M_1 \phi\right] + O(\varepsilon^7) \quad . \quad (55)$$

Introducing this into the balance equation (30), we obtain

$$-\frac{\varepsilon}{3} M_1 \phi - \frac{4\varepsilon^3}{45} M_1 \sigma_{a2}^{-1} M_1 \phi - \varepsilon^5 M_1 \sigma_{a2}^{-1} \left(\frac{16}{675} M_1 + \frac{4}{175} M_3\right) \sigma_{a2}^{-1} M_1 \phi + \frac{1}{c} (\sigma_t - \sigma_{,0}) \phi = \varepsilon q + O(\varepsilon^7) \quad . \quad (56)$$

This is a sixth-order partial differential equation for  $\phi$ . It is asymptotically equivalent to the transport equation (26) with  $O(\varepsilon^7)$  error.

Now we shall show that the  $SP_N$  equations asymptotically agree with Eq. (56) through terms of order  $\varepsilon^{2N+1}$ . To do this, we first ignore terms in Eq. (56) of  $O(\varepsilon^3)$  and obtain

$$-\frac{\partial}{\partial x_i} \left(\frac{\varepsilon}{3} \sigma_{a1}^{-1}\right) \frac{\partial}{\partial x_i} \phi_0 + \frac{1}{\varepsilon} \sigma_{a0} \phi_0 = \varepsilon q \quad . \quad (57)$$

Using Eqs. (20)-(22) and (49), we see that this is identical to the multigroup  $P_1$  equations (8). Thus, the multigroup  $P_1$  equations are an asymptotic approximation to the transport equation, with an  $O(\varepsilon^3)$  error.

Next, we ignore terms in Eq. (56) of  $O(\varepsilon^5)$  and obtain

$$-\left(I + \frac{4\varepsilon^2}{15} M_1 \sigma_{a2}^{-1}\right) \left(\frac{\varepsilon}{3} M_1\right) \phi + \frac{1}{\varepsilon} \sigma_{a0} \phi = \varepsilon q + O(\varepsilon^5) \quad , \quad (58)$$

or

$$-\left(I - \frac{4\varepsilon^2}{15} M_1 \sigma_{a2}^{-1}\right)^{-1} \left(\frac{\varepsilon}{3} M_1\right) \phi + \frac{1}{\varepsilon} \sigma_{a0} \phi = \varepsilon q + O(\varepsilon^5) \quad . \quad (59)$$

Hence, dropping the error term,

$$-\frac{\varepsilon}{3}M_1\phi + \left(I - \frac{4\varepsilon^2}{15}M_1\sigma_{a2}^{-1}\right) \left(\frac{1}{\varepsilon}\sigma_{a0}\phi - \varepsilon q\right) = 0 \quad , \quad (60)$$

or

$$-\frac{\varepsilon}{3}M_1 \left[ \phi + \frac{4\varepsilon}{5}\sigma_{a2}^{-1} \left( \frac{1}{\varepsilon}\sigma_{a0}\phi - \varepsilon q \right) \right] + \frac{1}{\varepsilon}\sigma_{a0}\phi = \varepsilon q \quad . \quad (61)$$

Using Eqs. (20)-(22) and (49), we see that this is identical to the multigroup SP<sub>2</sub> equations (13). Thus, the multigroup SP<sub>2</sub> equations are an asymptotic approximation to the transport equation with an error of O(ε<sup>5</sup>), provided that the physical system is homogeneous or the solution has sufficiently weak tangential derivatives at material interfaces. (This proviso is not needed for the multigroup P<sub>1</sub> equations.)

Finally, we ignore terms in Eq. (56) of O(ε<sup>7</sup>). The resulting equation may be written

$$-\frac{\varepsilon}{3}M_1(\phi + 2\phi_2) + \frac{1}{\varepsilon}\sigma_{a0}\phi = \varepsilon q \quad , \quad (62)$$

where

$$\begin{aligned} \phi_2 &= \left[ I + \varepsilon^2\sigma_{a2}^{-1} \left( \frac{4}{15}M_1 + \frac{9}{35}M_3 \right) \right] \frac{2\varepsilon^2}{15}\sigma_{a2}^{-1}M_1\phi + O(\varepsilon^6) \\ &= \left[ I - \varepsilon^2\sigma_{a2}^{-1} \left( \frac{4}{15}M_1 + \frac{9}{35}M_3 \right) \right]^{-1} \frac{2\varepsilon^2}{15}\sigma_{a2}^{-1}M_1\phi + O(\varepsilon^6) \quad . \end{aligned} \quad (63)$$

Dropping the error term, we may rewrite Eq. (63) as

$$\left[ I - \varepsilon^2\sigma_{a2}^{-1} \left( \frac{4}{15}M_1 + \frac{9}{35}M_3 \right) \right] \phi_2 = \frac{2\varepsilon^2}{15}\sigma_{a2}^{-1}M_1\phi \quad . \quad (64)$$

Multiplying by σ<sub>a2</sub>/ε, rearranging, and using Eq. (62), we obtain

$$-\frac{9\varepsilon}{35}M_3\phi_2 + \frac{1}{\varepsilon}\sigma_{a2}\phi_2 = \frac{2}{5} \left[ \frac{\varepsilon}{3}M_1(\phi + 2\phi_2) \right] = \frac{2}{5} \left( \frac{1}{\varepsilon}\sigma_{a0}\phi - \varepsilon q \right) \quad . \quad (65)$$

Using Eqs. (20)-(22) and (49), we see that Eqs. (62) and (65) are identical to the multigroup SP<sub>3</sub> equations (18) and (19). Thus, the multigroup SP<sub>3</sub> equations are an asymptotic approximation to the transport equation with an error of O(ε<sup>7</sup>), provided that the physical system is homogeneous or the solution has sufficiently weak tangential derivatives at material interfaces.

#### IV. NUMERICAL RESULTS

In this section give a computational comparison of the multigroup P<sub>1</sub>, SP<sub>3</sub>, and S<sub>4</sub> methods with anisotropic scattering for calculating the k-eigenvalue of a small supercritical sphere of uranium. The uranium has a density of 37.4 g/cm<sup>3</sup> and is composed of the isotopes U<sup>234</sup>, U<sup>235</sup>, and U<sup>238</sup>, with atomic fractions of 0.001054, 0.93737, and 0.05209, respectively. The sphere has a radius of 6.9355 cm. All calculations were performed with NIKE, a 3-D even-parity unstructured tetrahedral-mesh code which offers options for both the S<sub>N</sub> and SP<sub>N</sub> methods. The sphere was modeled with 2587 nodes and 13,120 tetrahedra. All of the calculations were performed on the massively-parallel Connection Machine-200 computer at LANL using a 12-group P<sub>1</sub> set of MENDEF-5 cross-sections.<sup>23</sup>

The computational results are given in Table 1. (We also calculated a benchmark result for k<sub>eff</sub> using a 1-D spherical geometry transport code with an extremely fine spatial mesh and the S<sub>100</sub> quadrature set; the resulting eigenvalue is k<sub>eff</sub> = 1.3923, which is very close to the S<sub>4</sub> value given in Table 1.) It can be seen that the SP<sub>3</sub> eigenvalue differs from the S<sub>4</sub> eigenvalue by about one percent, whereas the P<sub>1</sub> eigenvalue differs from the S<sub>4</sub> eigenvalue by about five percent. Comparing CPU times, we find that the SP<sub>3</sub> method is about four times faster than the S<sub>4</sub>

method. Although the  $P_1$  method appears to be less than twice as fast as the  $SP_3$  method, the particular solution algorithm used in NIKE is not optimal for the  $P_1$  method and runs about twice as long as an optimal algorithm would. Thus, an optimal  $P_1$  method would be about three times faster than the  $SP_3$  method. Overall, our  $SP_N$  results behave as expected. For the problem considered, the  $SP_3$  solution is much more accurate than the diffusion ( $P_1$ ) solution, but much less costly than the  $S_4$  solution method.

Method	$k_{eff}$	CPU Time (s)
$P_1$	1.328	211
$SP_3$	1.408	300
$S_4$	1.390	1351

Table 1:  $P_1$ ,  $SP_2$ , and  $S_4$  Eigenvalues

#### IV. DISCUSSION

In this paper, we have shown that if the multigroup neutron transport equation with anisotropic scattering is considered for problems in which, for  $\epsilon \ll 1$ ,

1. the physical system is  $O(\epsilon^{-1})$  mean free paths thick,
2. the probability of absorption is  $O(\epsilon^2)$ ,
3. the mean scattering cosine is not close to unity,

then:

1. the  $P_1$  equations are an asymptotic approximation to the transport equation with error  $O(\epsilon^3)$ ,
2. the  $SP_2$  and  $SP_3$  equations are an asymptotic approximation to the transport equation with respective errors  $O(\epsilon^5)$  and  $O(\epsilon^7)$ , provided that either (i) the physical system is homogeneous or (ii) the system is heterogeneous, and the transport solution has weak tangential derivatives at material interfaces.

Therefore, the  $SP_N$  equations can be understood as asymptotic corrections to  $P_1$  theory. Also, for planar geometry problems, they exactly reduce to the  $P_N$  (or,  $S_{N+1}$ ) equations. In practice, the  $SP_N$  solutions are most accurate for problems that are reasonably close to ones that could be called "diffusive," or for problems that have transport regions in which the solution behaves nearly one-dimensionally. (This latter case of course includes all one dimensional geometries.) For problems that have strong multidimensional transport effects, such as voids, with streaming regions, or geometrically complex spatial inhomogeneities, the  $SP_N$  solutions are less accurate.

In general, if a transport problem is one in which the standard diffusion or  $P_1$  approximation is *reasonably* accurate (but perhaps not as accurate as desired), then the  $SP_N$  approximations should be significantly more accurate (i.e., transport-like). This is the general observation of researchers who have experimented numerically with the  $SP_N$  equations, and it is consistent with our asymptotic theory. Thus, used for the proper kinds of problems,  $SP_N$  theory can be an accurate and relatively inexpensive way of including additional transport physics in a conventional diffusion code.

#### ACKNOWLEDGEMENTS

The work by the first author (E.W.L.) was supported by the NSF grant ECS-9107725. The work by the second and third authors (J.E.M. and J.M.M.) was performed under the auspices of the U.S. Department of Energy.

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