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# ASYMPTOTIC DERIVATION OF THE SIMPLIFIED $\mathrm{P_N}$ EQUATIONS

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## ABSTRACT

The diffusion and simplified $\mathrm{P_N}$ equations are derived from the transport equation by means of an asymptotic expansion in which the diffusion equation is the leading order approximation and the simplified $\mathrm{P_N}$ equations are higher-order approximations. In addition, the simplified $\mathrm{P_N}$ equations are reformulated in a "canonical" form that greatly facilitates the formulation of boundary conditions and the implementation of the resulting problem in a conventional multigroup diffusion code. Numerical comparisons of $\mathrm{S_N}$, diffusion, and simplified $\mathrm{P_N}$ solutions show that the simplified $\mathrm{P_N}$ solutions often contain most of the transport corrections for the diffusion approximation.

## I. INTRODUCTION

The spherical harmonic or $\mathrm{P_N}$ equations have been a well-known and widely-used approximation to the transport equation for the past 50 years. This approximation has the following properties:

1. The angularly-dependent transport equation is replaced by a finite system of equations in which the angular variable is explicitly absent.
2. As the order $N$ of the approximation increases, one recovers the exact transport solution.
3. The $\mathrm{P_N}$ equations are rotationally invariant; their solutions are free of ray effects.
4. In three-dimensional geometry, the number of $\mathrm{P_N}$ equations equals $N^2$. In planar geometry, the number of $\mathrm{P_N}$ equations is only $N$.
5. For $N > 1$, the $\mathrm{P_N}$ equations are not known to have a positive solution.

To deal with the large number and complexity of the $\mathrm{P_N}$ equations, Gelbard[1–3,10] and other researchers[4–9,11–15] have proposed a "simplified $\mathrm{P_N}$" ($\mathrm{SP_N}$) approximation in which the number of equations equals $N$ (hence is significantly less than with the multidimensional $\mathrm{P_N}$ equations), but one abandons the requirement that the exact transport solution is obtained as $N \to \infty$. Instead, the goal is to obtain a relatively inexpensive generalization of diffusion theory that contains most of the transport physics lacking in diffusion theory. Presently, the $SP_N$ equations have an incomplete theoretical foundation. Nevertheless, they have been tested in 1-D as well as 2-D and 3-D problems, and the reported numerical results are impressive. For many problems, low-order $SP_N$ equations capture most (Gamino[13] reports "greater than 80%") of the transport corrections to the diffusion approximation.

In this paper, we show that the $SP_N$ equations are robust high-order asymptotic approximations of the transport equation in a physical regime in which the conventional $P_1$ equations are the leading-order approximation. In other words, $SP_N$ theories contain higher-order asymptotic corrections to $P_1$ theory. This explains the high accuracy often exhibited by numerical solutions of the $SP_N$ equations.

We also reformulate the $SP_3$ equations in a new "canonical" form. For planar-geometry problems, this form reduces to the second-order even-parity $S_N$ equations, and for general isotropic scattering problems, it reduces to a conventional system having the form of multigroup diffusion equations. Because of these properties, the canonical form (*i*) makes the question of boundary conditions for these equations almost trivial, (*ii*) greatly facilitates the implementation of the $SP_3$ problem in a standard multigroup diffusion code, and (*iii*) shows that for a proper choice of boundary conditions, the solutions of the $SP_3$ equations are positive. This canonical form can be obtained for any odd-order system of $SP_N$ equations.

Finally, we present multidimensional numerical results obtained from a test code utilizing the canonical form of the $SP_N$ equations. As earlier work has shown, we find that low-order $SP_N$ solutions are a significant improvement over $P_1$ solutions and are obtained at a small fraction of the cost of an $S_N$ calculation.

The remainder of this paper is organized as follows. In Section II we asymptotically derive the $P_1$, $SP_2$, and $SP_3$ equations for the one-group transport equation with isotropic scattering. (Higher-order $SP_N$ equations can be derived by continuing this procedure.) In Section III, we reformulate the $SP_3$ equations into "canonical" form, and we propose boundary conditions for this new form. In Section IV we present numerical results. We conclude in Section V with a discussion.

## II. ASYMPTOTIC ANALYSIS

In this paper we shall consider the one-group three-dimensional transport equation with isotropic scattering:

$$\underline{\Omega} \cdot \underline{\nabla}\psi(\underline{r},\underline{\Omega}) + \Sigma_t(\underline{r})\psi(\underline{r},\underline{\Omega}) = \frac{\Sigma_s(\underline{r})}{4\pi}\int \psi(\underline{r},\underline{\Omega}')d\Omega' + \frac{Q(\underline{r})}{4\pi} \quad . \tag{1}$$

More complex (multigroup, anisotropic scattering) problems require a more complicated asymptotic analysis that we will present elsewhere. We consider Eq. (1) under the scaling:

$$\Sigma_t(\underline{r}) = \frac{\sigma_t(\underline{r})}{\varepsilon} \quad , \tag{2}$$

$$\Sigma_a(\underline{r}) = \varepsilon\sigma_a(\underline{r}) \quad , \tag{3}$$

$$\Sigma_s(\underline{r}) = \Sigma_t(\underline{r}) - \Sigma_a(\underline{r}) = \frac{\sigma_t(\underline{r})}{\varepsilon} - \varepsilon\sigma_a(\underline{r}) \quad , \tag{4}$$

$$Q(\underline{r}) = \varepsilon q(\underline{r}) \quad , \tag{5}$$

where $\sigma_t$, $\sigma_a$, and $q$ are $O(1)$ and $\varepsilon \ll 1$. The physics implied by this scaling is:

1. The system is optically thick ($\Sigma_t \gg 1$).

2. The rates of absorption and production due to interior sources are comparable and weak [$\Sigma_a = O(\varepsilon)$ and $Q = O(\varepsilon)$].
3. The infinite medium solution $\phi = Q/\Sigma_a = q/\sigma_a$ is $O(1)$.
4. The diffusion length $L = (3\Sigma_t\Sigma_a)^{-1/2} = (3\sigma_t\sigma_a)^{-1/2}$ is $O(1)$.
5. If one introduces the scaling defined by Eqs. (2)-(5) into the standard diffusion approximation to Eq. (1), the resulting equation is independent of $\varepsilon$. In other words, the standard diffusion equation is invariant under the scaling (2)-(5).

The scaling defined by Eqs. (2)-(5) has long been known[16,17] to be one in which transport theory asymptotically transitions into diffusion theory as $\varepsilon \to 0$. In this paper, we show that higher-order asymptotic corrections to diffusion theory yield simplified $\mathrm{P_N}$ theories.

To begin, we introduce Eqs. (2)-(5) into Eq. (1) and multiply by $\varepsilon/\sigma_t$ to get

$$\left(I + \frac{\varepsilon}{\sigma_t}\underline{\Omega}\cdot\underline{\nabla}\right)\psi = \frac{1}{4\pi}\left[\left(1 - \varepsilon^2\frac{\sigma_a}{\sigma_t}\right)\phi + \varepsilon^2\frac{q}{\sigma_t}\right] \quad , \tag{6}$$

where

$$\phi(\underline{r}) = \int \psi(\underline{r},\underline{\Omega}')d\Omega' \quad . \tag{7}$$

Next, we invert the operator on the left side of Eq. (6) and integrate over $\underline{\Omega}$ to obtain the Peierls integral equation for the scalar flux:

$$\phi = \left[\frac{1}{4\pi}\int\left(I + \frac{\varepsilon}{\sigma_t}\underline{\Omega}\cdot\underline{\nabla}\right)^{-1}d\Omega\right]\left[\left(1 - \varepsilon^2\frac{\sigma_a}{\sigma_t}\right)\phi + \varepsilon^2\frac{q}{\sigma_t}\right] \quad . \tag{8}$$

If there are non-vacuum boundary conditions, then extra terms occur in Eq. (8). However, these are $O(e^{-\rho/\varepsilon})$, where $\rho$ is the optical distance to the boundary. Thus, in the interior of the system these terms are exponentially small and we will ignore them.

Next, we formally expand the operator on the right side of Eq. (8) in powers of $\varepsilon$. We obtain

$$\phi = \left(\sum_{n=0}^{\infty}\varepsilon^{2n}\mathcal{L}_{2n}\right)\left[\left(1 - \varepsilon^2\frac{\sigma_a}{\sigma_t}\right)\phi + \varepsilon^2\frac{q}{\sigma_t}\right] \quad , \tag{9}$$

where

$$\mathcal{L}_{2n} = \frac{1}{4\pi}\int\left(\frac{1}{\sigma_t}\underline{\Omega}\cdot\underline{\nabla}\right)^{2n}d\Omega \quad . \tag{10}$$

The operators $\mathcal{L}_0$, $\mathcal{L}_2$, and $\mathcal{L}_4$ are explicitly defined by

$$\mathcal{L}_0 = I \quad , \tag{11}$$

$$\mathcal{L}_2 = \frac{1}{3}\sum_{i,j=1}^{3}(\delta_{ij})\left(\frac{1}{\sigma_t}\frac{\partial}{\partial x_i}\frac{1}{\sigma_t}\frac{\partial}{\partial x_j}\right) = \frac{1}{\sigma_t}\underline{\nabla}\cdot\frac{1}{3\sigma_t}\underline{\nabla} \quad , \tag{12}$$

$$\mathcal{L}_4 = \frac{1}{15}\sum_{i,j,k,l=1}^{3}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\left(\frac{1}{\sigma_t}\frac{\partial}{\partial x_i}\frac{1}{\sigma_t}\frac{\partial}{\partial x_j}\frac{1}{\sigma_t}\frac{\partial}{\partial x_k}\frac{1}{\sigma_t}\frac{\partial}{\partial x_l}\right) \quad . \tag{13}$$

If the system is homogeneous or the problem has spatial variation in only one direction, the formulas for $\mathcal{L}_{2n}$, $n \geq 2$, simplify to:

$$\mathcal{L}_{2n} = \frac{3^n}{2n+1}\left(\mathcal{L}_2\right)^n \quad . \tag{14}$$

In our analysis, we shall replace the original definition of $\mathcal{L}_{2n}$ [Eq. (10)] by Eq. (14). This is rigorously correct for a homogeneous system or for a spatially one-dimensional problem, but not for a true multidimensional problem at material interfaces. We shall discuss this approximation again in Sec. V.

Introducing Eq. (14) into Eq. (9), we get

$$\phi = \left( I + \varepsilon^2 \mathcal{L}_2 + \frac{9\varepsilon^4}{5} \mathcal{L}_2^2 + \frac{27\varepsilon^6}{7} \mathcal{L}_2^3 + O\left(\varepsilon^8\right) \right) \left[ \left( 1 - \varepsilon^2 \frac{\sigma_a}{\sigma_t} \right) \phi + \varepsilon^2 \frac{q}{\sigma_t} \right] \quad . \tag{15}$$

Formally inverting the operator on the right side of this equation, we obtain:

$$\left( I - \varepsilon^2 \mathcal{L}_2 - \frac{4\varepsilon^4}{5} \mathcal{L}_2^2 - \frac{44\varepsilon^6}{35} \mathcal{L}_2^3 + O\left(\varepsilon^8\right) \right) \phi = \left( 1 - \varepsilon^2 \frac{\sigma_a}{\sigma_t} \right) \phi + \varepsilon^2 \frac{q}{\sigma_t} \quad , \tag{16}$$

or

$$-\sigma_t \left( \mathcal{L}_2 \phi + \frac{4\varepsilon^2}{5} \mathcal{L}_2^2 \phi + \frac{44\varepsilon^4}{35} \mathcal{L}_2^3 \phi + O\left(\varepsilon^6\right) \right) + \sigma_a \phi = q \quad . \tag{17}$$

If we now retain terms of $O(\varepsilon^{2n})$ but discard all higher order terms, we obtain a partial differential equation for $\phi$ of order $2n$. This equation is an asymptotic approximation to the Peierls equation (8), but it is not any of the simplified $\mathrm{P_N}$ approximations. To derive these approximations, we must rewrite the equation obtained from Eq. (17) in an asymptotically equivalent form as either a single second-order equation or as a coupled system of second-order equations. We shall now give the details of this procedure.

### II.1 Diffusion ($\mathbf{P_1}$) Equation

We delete terms of $O(\varepsilon^2)$ and higher in Eq. (17) and use the definition (12) to get

$$-\underline{\nabla} \cdot \frac{1}{3\sigma_t} \underline{\nabla} \phi + \sigma_a \phi = q \quad . \tag{18}$$

Multiplying this equation by $\varepsilon$ and using the definitions (2)-(5), we obtain

$$-\underline{\nabla} \cdot \frac{1}{3\Sigma_t(\underline{r})} \underline{\nabla} \phi(\underline{r}) + \Sigma_a(\underline{r}) \phi(\underline{r}) = Q(\underline{r}) \quad . \tag{19}$$

This is the conventional diffusion ($\mathrm{P_1}$) equation.

### II.2 Simplified $\mathbf{P_2}$ Equation

We delete terms of $O(\varepsilon^4)$ and higher in Eq. (17) and rearrange slightly to get

$$\left( I + \frac{4\varepsilon^2}{5} \mathcal{L}_2 \right) \mathcal{L}_2 \phi = \frac{\sigma_a \phi - q}{\sigma_t} \quad . \tag{20}$$

Operating on this equation by $(I - 4\varepsilon^2 \mathcal{L}_2/5)$ and again deleting terms of $O(\varepsilon^4)$, we obtain

$$\mathcal{L}_2 \phi = \left( I - \frac{4\varepsilon^2}{5} \mathcal{L}_2 \right) \frac{\sigma_a \phi - q}{\sigma_t} \quad , \tag{21}$$

or, using Eq. (12),

$$-\underline{\nabla}\cdot\frac{1}{3\sigma_t}\underline{\nabla}\left(\phi+\frac{4\varepsilon^2}{5}\frac{\sigma_a\phi-q}{\sigma_t}\right)+\sigma_a\phi=q \quad . \tag{22}$$

Multiplying this equation by $\varepsilon$ and using the definitions (2)-(5), we obtain

$$-\underline{\nabla}\cdot\frac{1}{3\Sigma_t(\underline{r})}\underline{\nabla}\left(\phi(\underline{r})+\frac{4}{5}\frac{\Sigma_a(\underline{r})\phi(\underline{r})-Q(\underline{r})}{\Sigma_t(\underline{r})}\right)+\Sigma_a(\underline{r})\phi(\underline{r})=Q(\underline{r}) \quad . \tag{23}$$

This is the $SP_2$ equation.

### II.3 Simplified $P_3$ Equations

Now we delete terms of $O(\varepsilon^6)$ in Eq. (17) to obtain

$$-\sigma_t\mathcal{L}_2\left(\phi+\frac{4\varepsilon^2}{5}\mathcal{L}_2\phi+\frac{44\varepsilon^4}{35}\mathcal{L}_2^2\phi\right)+\sigma_a\phi=q \quad . \tag{24}$$

Hence, if we define

$$\xi(\underline{r})=\frac{2\varepsilon^2}{5}\mathcal{L}_2\phi(\underline{r})+\frac{22\varepsilon^4}{35}\mathcal{L}_2^2\phi(\underline{r})=\left(I+\frac{11\varepsilon^2}{7}\mathcal{L}_2\right)\frac{2\varepsilon^2}{5}\mathcal{L}_2\phi(\underline{r}) \quad , \tag{25}$$

then Eq. (24) can be written

$$-\sigma_t\mathcal{L}_2\left(\phi+2\xi\right)+\sigma_a\phi=q \quad . \tag{26}$$

Operating on Eq. (25) by $(I-11\varepsilon^2\mathcal{L}_2/7)$ and again deleting terms of $O(\varepsilon^6)$, we get

$$\left(-\frac{11\varepsilon^2}{7}\mathcal{L}_2+I\right)\xi=\frac{2\varepsilon^2}{5}\mathcal{L}_2\phi \quad . \tag{27}$$

Now, multiplying Eq. (26) by $\varepsilon$ and using the definitions (2)-(5) and (12), we obtain

$$-\underline{\nabla}\cdot\frac{1}{3\Sigma_t(\underline{r})}\underline{\nabla}\left[\phi(\underline{r})+2\xi(\underline{r})\right]+\Sigma_a(\underline{r})\phi(\underline{r})=Q(\underline{r}) \quad . \tag{28}$$

Likewise, multiplying Eq. (27) by $\sigma_t/\varepsilon$ and using the definitions (2)-(5) and (12), we obtain

$$-\underline{\nabla}\cdot\frac{1}{3\Sigma_t(\underline{r})}\underline{\nabla}\left[\frac{11}{7}\xi(\underline{r})+\frac{2}{5}\phi(\underline{r})\right]+\Sigma_t(\underline{r})\xi(\underline{r})=0 \quad . \tag{29}$$

Eqs. (28) and (29) are the $SP_3$ equations.

We note that the three-dimensional $P_1$, $SP_2$, and $SP_3$ results derived above could have been obtained by the following ad-hoc procedure:

1. Write the planar-geometry $P_N$ approximations to Eq. (1) in second order form (i.e., eliminate the odd angular flux moments).

2. Replace the one-dimensional diffusion operator by its three-dimensional generalization:

$$\left(\frac{d}{dx}\frac{1}{\Sigma_t}\frac{d}{dx}\right)\rightarrow\left(\underline{\nabla}\cdot\frac{1}{\Sigma_t}\underline{\nabla}\right) \quad . \tag{30}$$

This, in fact, is the procedure that has previously been used to derive the $SP_N$ equations. The asymptotic analysis presented above, which can easily be extended to higher-order $SP_N$ approximations, legitimizes the results of this procedure by showing that for certain problems, the $SP_N$ equations are an asymptotic approximation to the transport equation. The problems for which this is *strictly* true are ones for which Eq. (14) holds for $n \geq 2$, i.e.,

1. Multidimensional problems in a medium in which $\Sigma_t$ is constant (but $\Sigma_s$ can vary).

2. One-dimensional problems in an inhomogeneous medium.

The problems for which this is *approximately* true are:

1. Truly diffusive problems, in which $\mathcal{L}_{2n}\phi \approx 0$ for $n \geq 2$. (For these problems, the higher-order asymptotic corrections are negligible, so the approximations made in deriving them play no role.)

2. Multidimensional problems in inhomogeneous media for which the solution at interfaces is locally one-dimensional in the direction normal to the interface.

Thus, for multidimensional heterogeneous nondiffusive problems, the $SP_N$ equations for $n \geq 2$ are not strict asymptotic approximations to the transport equation. However, they are very closely related to asymptotic approximations, and numerical calculations show that in many problems, they contain most of the transport physics that is lacking in the $P_1$ approximation.

## III. CANONICAL FORM OF THE $SP_3$ EQUATIONS

We now rewrite Eqs. (28) and (29) in "canonical" form. To do this, we multiply Eq. (29) by a constant $\lambda$ and add the result to Eq. (28). This yields

$$-\underline{\nabla} \cdot \frac{1}{\Sigma_t} \underline{\nabla} \left[ \frac{\phi + 2\xi}{3} + \lambda \left( \frac{2\phi}{15} + \frac{11\xi}{21} \right) \right] + \Sigma_t \left( \phi + \lambda\xi \right) = \Sigma_s \phi + Q \quad . \tag{31}$$

Now we seek constants $\mu^2$ and $\lambda$ such that for arbitrary functions $\phi(\underline{r})$ and $\xi(\underline{r})$,

$$\frac{\phi + 2\xi}{3} + \lambda \left( \frac{2\phi}{15} + \frac{11\xi}{21} \right) = \mu^2 \left( \phi + \lambda\xi \right) \quad . \tag{32}$$

We easily obtain two solutions; for $n = 1$ and 2,

$$\mu_n^2 = \frac{15 + (-1)^n 2\sqrt{30}}{35} \quad : \quad \mu_1 \approx 0.340 \quad , \quad \mu_2 \approx 0.861 \quad , \tag{33}$$

$$\lambda_n = \frac{5}{2} \left( 3\mu_n^2 - 1 \right) \quad : \quad \lambda_1 \approx -1.633 \quad , \quad \lambda_2 \approx 3.061 \quad . \tag{34}$$

Hence, if we define

$$\psi_n(\underline{r}) = \phi(\underline{r}) + \lambda_n \xi(\underline{r}) \quad , \quad n = 1, 2 \quad , \tag{35}$$

then Eqs. (31) and (32) imply

$$-\underline{\nabla} \cdot \frac{\mu_n^2}{\Sigma_t} \underline{\nabla} \psi_n + \Sigma_t \psi_n = \Sigma_s \phi + Q \quad , \quad n = 1, 2 \quad . \tag{36}$$

Also, if we define

$$w_1 = \frac{\lambda_2}{\lambda_2 - \lambda_1} \approx 0.652 \quad , \quad w_2 = \frac{\lambda_1}{\lambda_1 - \lambda_2} \approx 0.348 \quad , \tag{37}$$

then

$$\phi(\underline{r}) = \psi_1(\underline{r})w_1 + \psi_2(\underline{r})w_2 \quad , \tag{38}$$

and Eqs. (36) can be written

$$-\underline{\nabla} \cdot \frac{\mu_n^2}{\Sigma_t(\underline{r})}\underline{\nabla}\psi_n(\underline{r}) + \Sigma_t(\underline{r})\psi_n(\underline{r}) = \Sigma_s(\underline{r})\sum_{m=1}^{2}\psi_m(\underline{r})w_m + Q(\underline{r}) \quad , \quad n = 1, 2 \quad . \tag{39}$$

This is the "canonical" form of the $SP_3$ equations. The constants $\mu_n$, $w_n$ in these equations constitute the usual planar-geometry $S_4$ Gauss-Legendre quadrature set. Therefore, in planar geometry, the canonical $SP_3$ equations reduce to the even-parity $S_4$ equations. In general geometry, the canonical $SP_3$ equations (with isotropic scattering) take the form of two-group diffusion equations with upscattering.

Eqs. (39) could have been obtained from Eq. (1) by the following ad-hoc procedure:

1. Write the planar-geometry even-parity $S_4$ approximation to Eq. (1) using the $S_4$ Gauss-Legendre quadrature set:

$$-\frac{d}{dx}\frac{\mu_n^2}{\Sigma_t}\frac{d}{dx}\psi_n + \Sigma_t\psi_n = \Sigma_s\sum_{m=1}^{2}\psi_m w_m + Q \quad , \quad n = 1, 2 \quad . \tag{40}$$

2. Make the same operator replacement as shown in Eq. (30), i.e.,

$$\left(\frac{d}{dx}\frac{1}{\Sigma_t}\frac{d}{dx}\right) \to \left(\underline{\nabla} \cdot \frac{1}{\Sigma_t}\underline{\nabla}\right) \quad . \tag{41}$$

Eqs. (39) are algebraically equivalent to the the $SP_N$ equations for the following reason. The planar geometry even-parity $S_4$ equations (40) are algebraically equivalent to the planar geometry $P_3$ equations. Thus, introducing the operator replacement (41) in Eqs. (40), we obtain Eqs. (39), and introducing the same operator replacement in the planar geometry $P_3$ equations, we obtain Eqs. (28) and (29).

We now turn to the question of boundary conditions for Eqs. (39). In principle, one could derive $SP_3$ boundary conditions using a high-order asymptotic boundary layer analysis, but this leads to a very complex result that is difficult to implement. Instead, we shall invoke the following "one-dimensional" principle: because Eqs. (39) reduce to the even-parity $S_4$ equations (40) for planar geometry problems, the boundary conditions for Eqs. (39) should reduce to the standard even-parity $S_4$ boundary conditions for planar geometry problems. For multidimensional problems in which the solutions have a locally one-dimensional character near the boundary, this principle seems reasonable and intuitive.

Thus, for $\underline{r}$ a point on the outer boundary with $\underline{n}$ the unit outer normal, reflecting boundary conditions that satisfy the one-dimensional principle are

$$\underline{n} \cdot \underline{\nabla}\psi_n(\underline{r}) = 0 \quad , \quad n = 1, 2 \quad . \tag{42}$$

Also, for $\underline{r}$ a boundary point at which an incident flux $f(\underline{r}, \underline{\Omega})$ is prescribed for $\underline{\Omega} \cdot \underline{n} < 0$, boundary conditions that satisfy the one-dimensional principle are

$$f_n(\underline{r}) = \psi_n(\underline{r}) + \frac{\mu_n}{\Sigma_t(\underline{r})}\underline{n} \cdot \underline{\nabla}\psi_n(\underline{r}) \quad , \quad n = 1, 2 \quad . \tag{43}$$

Here we have defined

$$f_1(\underline{r}) = \frac{1}{\mu_1 w_1}\int_{0<-\underline{\Omega}\cdot\underline{n}<w_1} |\underline{\Omega} \cdot \underline{n}|\, f(\underline{r}, \underline{\Omega})d\Omega \quad , \tag{44}$$

$$f_2(\underline{r}) = \frac{1}{\mu_2 w_2} \int\limits_{w_1 < -\underline{\Omega}\cdot\underline{n} < 1} \left|\underline{\Omega}\cdot\underline{n}\right| f(\underline{r},\underline{\Omega}) d\Omega \quad . \tag{45}$$

We note that $f_1$ and $f_2$ are proportional to the incoming partial currents over the angular "cones" that correspond to $\mu_1$ and $\mu_2$. The definition of these functions ensures that

$$\sum_{n=1}^{2} \mu_n f_n(\underline{r}) w_n = \int\limits_{\underline{\Omega}\cdot\underline{n}<0} \left|\underline{\Omega}\cdot\underline{n}\right| f(\underline{r},\underline{\Omega}) d\Omega \quad . \tag{46}$$

Therefore, for one-dimensional and multidimensional problems that behave in a locally one-dimensional manner near the outer boundary, the total incoming partial current is preserved.

We have shown that the canonical $SP_3$ equations are useful for prescribing boundary conditions. However, these equations have other important advantages:

1. They can easily be implemented in a conventional multigroup diffusion code.

2. Because solutions of standard multigroup diffusion problems are guaranteed to be positive, this is also true for solutions of multigroup diffusion $SP_3$ problems. This guarantee does not exist for solutions of standard $SP_3$ problems (with boundary conditions that are not equivalent to those given above) or of conventional $P_3$ problems.

3. The $SP_3$ equations are tightly coupled and often require acceleration for efficient solution. However, the canonical $SP_3$ equations, which so closely resemble the even-parity $S_4$ equations, can easily make use of diffusion acceleration procedures that apply to the even-parity $S_4$ equations[18]. Lack of space prevents a full discussion of this here.

The procedure described above can easily be applied to higher order $SP_N$ appproximations. For example, the canonical $SP_5$ equations take the form of a three-group diffusion problem with boundary conditions that are patterned after Eqs. (42)-(45). For planar geometry, these equations reduce to the conventional even-parity $S_6$ equations.

## IV. NUMERICAL RESULTS

First we shall consider two 3-D $k$-eigenvalue test problems for which the conventional diffusion solutions are inaccurate. These problems utilize a 3-D 2-group model of a small light-water reactor containing a core, a reflector and a control rod. They are described as Model 1, Case 1 (control rod out) and Model 1, Case 2 (control rod in) in the benchmark problems compiled by Takeda and Ikeda[19]. We solved these problems using the NIKE code[20,21], with a uniform 1.0 $cm^3$ mesh, on the CM2 computer at Los Alamos National Laboratory. The diffusion, canonical $SP_N$, and $S_4$ eigenvalues and running times are plotted in Figure 1.

We see that for both problems, the low-order canonical $SP_N$ calculations require significantly less computational time than the $S_4$ calculations. Also, the low-order $SP_N$ results for the "rod in" problem are significantly more accurate than the diffusion results. The $SP_N$ results for the "rod out" problem are more accurate than the diffusion results, but are less accurate than the "rod in" problem results. This is because the "rod out" problem contains a region with long neutron streaming paths. Hence, this problem contains transport effects that are not well-described by any diffusion or $SP_N$ approximation.

Next, we consider a 3-D problem in which classic ray effects are observed in $S_N$ solutions. This problem consists of a homogeneous, one-group, isotropically scattering 130 cm cube with $\sigma_t = 0.05$

cm$^{-1}$, $\sigma_s = 0.0025$ cm$^{-1}$ (c=0.05), six vacuum boundaries, and a uniform isotropic source in a 17.3 cm sub-cube situated in one corner. The system is depicted in Figure 2. In Figure 3, various $S_N$ and canonical $SP_N$ scalar fluxes are plotted along the line $x = 26$ cm, $z = 43.3$ cm, and $0 \le y \le 80$ cm. These results were also calculated with NIKE. Figure 3 shows that the $S_N$ solutions all contain ray effects, which tend to diminish as $N$ increases. However, the $SP_1$ (diffusion) and $SP_3$ solutions contain no ray effects, the diffusion solution is inaccurate, and the $SP_3$ solution agrees basically with the $S_{16}$ solution. (The $SP_5$ solution, which is not shown in the figure, agrees very closely with the $SP_3$ solution.)

We conclude that although $SP_N$ solutions do not limit to the exact transport solution as $N \to \infty$, they also do not contain the ray effect errors that are inherent in the $S_N$ equations, which *do* limit to the exact transport equation as $N \to \infty$.

## V. DISCUSSION

In this paper, we have derived the conventional and canonical $SP_N$ equations from the transport equation using a high-order asymptotic expansion in which the diffusion equation is the leading-order approximation and the $SP_N$ equations are higher-order approximations.

Problems in which the $SP_N$ equations are not accurate contain significant multidimensional heterogeneities that generate strong multidimensional space and angular variations in the angular flux. Problems in which the $SP_N$ equations are accurate are ones in which the multidimensional spatial and angular variations are weak, or if strong spatial and angular variations occur, they are locally one-dimensional in nature. This is depicted in Figure 4.

In summary, we have shown that the excellent numerical $SP_N$ results obtained by previous researchers is not accidental. The $SP_N$ equations are often just as theoretically valid an approximation of the transport equation as the $P_1$ equations, and as a practical matter, they are usually much more accurate. They should be useful in many problems for which conventional diffusion theory is not a sufficiently accurate approximation to transport theory.

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Figure 1: Model LWR Problems - Results

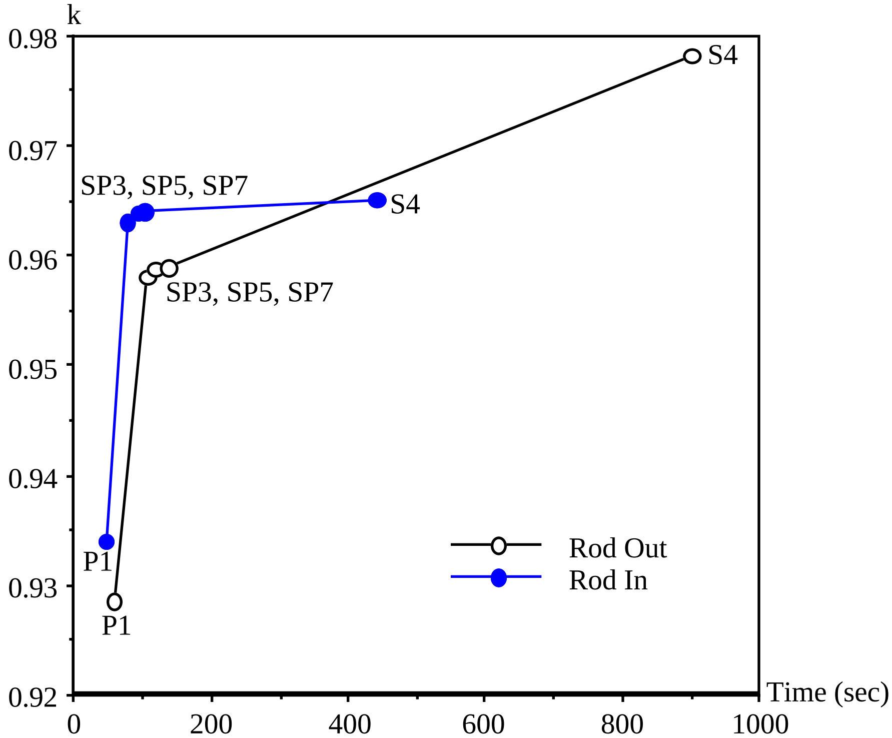


Figure 2: 3-D Ray Effect Problem (Geometry)

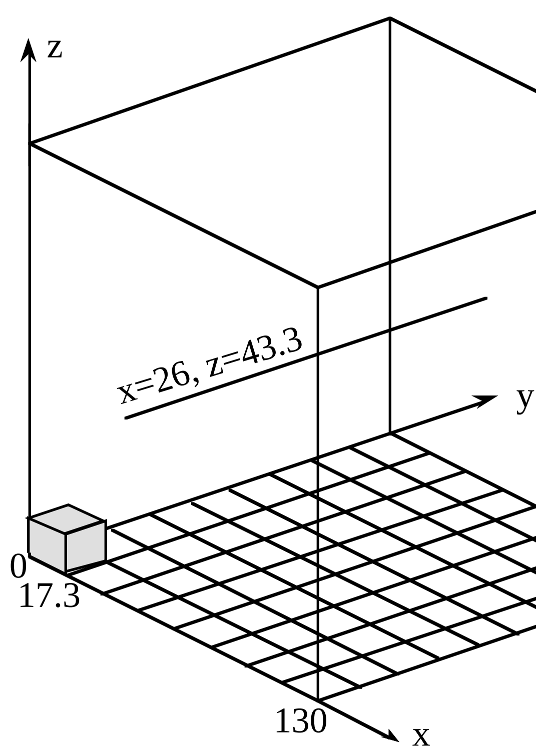

Figure 3: 3-D Ray Effect Problem ($S_N$ and $SP_N$ Scalar Fluxes)

Figure 4: Qualitative Performance of Diffusion and $SP_N$ Solutions
(Each theory is valid for problems that lie to the left of its curve.)