

A Computationally Viable Version of the P_N Method for Spheres

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Abstract — *The long-standing problem of implementing the P_N method effectively for spherical geometry is revisited in this work. It is shown that a least-squares approach to the method resolves to a great extent the numerical instability reported for the first time by Aronson in 1984. In the proposed version of the method, a small loss of accuracy is still observed for intermediate orders of the approximation, but in high order (typically $N \geq 199$), full accuracy is recovered, and the method can be used with confidence even for extremely high orders of the approximation. Numerical results of benchmark quality are tabulated for the quantities of interest for two basic transport problems in spherical geometry: the albedo problem for a sphere and the critical-sphere problem, both including cases that show the effects of scattering anisotropy described by the binomial law.*

Keywords — *Neutron transport, spherical geometry, spherical harmonics method.*

I. INTRODUCTION

The P_N method for solving transport problems in spherical geometry has attracted much attention along the years because of its simplicity and ability of treating, in an analytical way, the angular redistribution operator for spherically symmetric systems. In a paper published in 1947, Marshak¹ worked out the P_1 and P_3 approximations to the extrapolation distance (into an inner black sphere) for a purely scattering outer shell with external radius extending to infinity and reported numerical results obtained from the P_1 , P_3 , and P_5 approximations. Some years later, Davison included, as a chapter of his important book,² a derivation of the P_N method in spherical geometry for any order of the approximation. Davison's work focused on the theoretical aspects of the method. The numerical aspects of the method remained relatively unexplored until the mid-1980s, when Aronson^{3,4} showed

that the P_N method with either Marshak¹ or Federighi⁵ boundary conditions becomes numerically unstable for sufficiently large values of N when used to study neutron transport in spheres. Furthermore, Aronson observed that the onset of instability depends on the value of the radius of the sphere, occurring earlier (i.e., for lower values of N) the smaller the radius. In one of those papers³ source-driven problems are considered, while in the other⁴ the focus is on critical problems.

Shortly thereafter, two of the authors (CES and JRT) confirmed Aronson's observations for Marshak boundary conditions and found that singular-value decomposition (SVD) could be used to obtain improved numerical results from the P_N method with Marshak boundary conditions for spheres. However, it was concluded that even using SVD did not help in obtaining reference-quality results for cases defined by small radii or cases where large values of N were required. At that time (1985), this difficulty was attributed to the fact that small singular values kept appearing as N was increased in the

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calculations performed for such cases. However, in light of the present work, we now know that such a limitation could have been overcome by a judicious choice of the threshold below which a column of the matrix to be decomposed is discarded in SVD.

In this work, we show how a least-squares approach to the P_N method for spheres can be used to resolve, to a great extent, the instability problem reported by Aronson. In our implementation of the method, a small loss of accuracy is still observed for intermediate orders of the approximation, but in high order full accuracy is recovered, and the method can be used with confidence even for extremely high orders of the approximation. For example, in order to test the numerical limits of our solutions, we have gone as far as $N = 30999$ in FORTRAN double precision (DP) (approximately 16 decimal digits) when solving the problem studied in Sec. III and $N = 26999$ when solving the problem studied in Sec. IV.

With regard to solution methods, we note that in the past there have been two approaches used to solve, in a spatially continuous way, neutron transport or radiative transfer problems in spheres: (1) converting the integro-differential equation to an integral equation and making expansions in the spatial variable^{6,7} and (2) recasting the original problem to a pseudo problem⁸ that could be solved with classical methods, for example, the F_N method⁹⁻¹² or the P_N method.^{13,14} However, both of the mentioned approaches are severely limited in that highly anisotropic scattering laws and/or reflective boundary conditions cannot be (or at least have not been shown to be) solvable by these methods. For example, the process of converting the integro-differential equation for a sphere to an integral form leads not to a single equation but to a set (of the order of the scattering law) of integral equations—a hopeless situation for many-term scattering laws. The conversion of the original problem to a pseudo problem seems a rare miracle that has not been developed for anything but the simplest of problems. And so the current work is, to our knowledge, the first one that gives a procedure capable of yielding spatially and angularly continuous solutions for a very broad class of neutron transport and radiative transfer problems in spherical media and can accommodate, without any additional effort, anisotropic scattering of arbitrary order.

II. THE P_N METHOD IN SPHERICAL GEOMETRY

We consider the one-speed neutron transport equation for spherically symmetric systems, written as

$$\begin{aligned} &\mu \frac{\partial}{\partial r} \psi(r, \mu) + \frac{1 - \mu^2}{r} \frac{\partial}{\partial \mu} \psi(r, \mu) + \psi(r, \mu) \\ &= \frac{c}{2} \sum_{l=0}^L (2l + 1) f_l P_l(\mu) \int_{-1}^1 P_l(\mu') \psi(r, \mu') d\mu', \end{aligned} \quad (1)$$

where $\psi(r, \mu)$ is the angular flux, r is the radial distance measured in mean free paths from the origin, and $\mu = \Omega \cdot \mathbf{e}_r$, with Ω and \mathbf{e}_r denoting unit vectors, respectively, in the direction of neutron motion and in the radial direction. In addition, c is the mean number of secondary neutrons per collision and $\{f_l\}$, with $f_0 = 1$, are the coefficients of a truncated expansion of the scattering law in terms of the Legendre polynomials $\{P_l(\mu_0)\}$, with μ_0 denoting the cosine between the directions of neutron motion before and after a scattering event.

Introducing the P_N approximation

$$\psi(r, \mu) = \frac{1}{2} \sum_{n=0}^N (2n + 1) \phi_n(r) P_n(\mu) \quad (2)$$

with N odd into Eq. (1) and using some properties of the Legendre polynomials, we obtain the following set of ordinary differential equations for the Legendre moments $\{\phi_n(r)\}$:

$$\begin{aligned} &(n + 1) \left[\frac{d}{dr} + \frac{n + 2}{r} \right] \phi_{n+1}(r) \\ &+ n \left[\frac{d}{dr} - \frac{n - 1}{r} \right] \phi_{n-1}(r) + h_n \phi_n(r) = 0 \end{aligned} \quad (3)$$

for $n = 0, 1, \dots, N$. Here,

$$h_n = \begin{cases} (2n + 1)(1 - cf_n), & n = 0, 1, \dots, L, \\ 2n + 1, & n = L + 1, L + 2, \dots, N. \end{cases} \quad (4)$$

We note that for isotropic scattering ($L = 0$) Eq. (3) reduces to the set of differential equations studied by Davison² and by Case and Zweifel.¹⁵ Since our way of finding the solutions of Eq. (3) differs somewhat from that of Davison² and the notations are slightly different, we include some details of our derivation in the Appendix.

As shown in the Appendix, the general solution of Eq. (3) can be written as

$$\phi_n(r) = \sum_{j=1}^J \left[\tilde{A}_j k_n(r/\xi_j) + (-1)^n \tilde{B}_j i_n(r/\xi_j) \right] g_n(\xi_j), \quad (5)$$

for $n = 0, 1, \dots, N$. Here, $i_n(z)$ and $k_n(z)$ are, respectively, the modified spherical Bessel functions of the first and third kinds,¹⁶ $g_n(\xi)$ is the polynomial introduced by Chandrasekhar,¹⁷ $\{\xi_j\}$ are the P_N eigenvalues (see the Appendix for details), and $\{\tilde{A}_j\}$ and $\{\tilde{B}_j\}$ are unknown coefficients to be determined.

Finally, an explicit expression for the P_N approximation to the angular flux is obtained by substituting Eq. (5) into Eq. (2). We get

$$\psi(r, \mu) = \frac{1}{2} \sum_{n=0}^N (2n+1) P_n(\mu) \sum_{j=1}^J \left[\tilde{A}_j k_n(r/\xi_j) + (-1)^n \tilde{B}_j i_n(r/\xi_j) \right] g_n(\xi_j). \quad (6)$$

III. A SPHERE SUBJECT TO EXTERNAL NEUTRON INCIDENCE

In this section, we consider the problem of a sphere of radius R and $c \leq 1$ subject to a known distribution of incoming neutrons on its surface.

III.A. Formulation

The problem is formulated by Eq. (1) for $r \in (0, R)$ and $\mu \in [-1, 1]$ and the conditions

$$\psi(R, -\mu) = f(\mu), \quad (7a)$$

for $\mu \in (0, 1]$, and

$$\lim_{r \rightarrow 0} \psi(r, \mu) < \infty, \quad (7b)$$

for $\mu \in [-1, 1]$. The last condition is just a mathematical statement of the fact that the solution of this problem is not expected to diverge at the center of the sphere.

The quantity of most interest for this problem is the albedo (or reflection factor)

$$A^* = \left[\int_0^1 \mu \psi(R, -\mu) d\mu \right]^{-1} \int_0^1 \mu \psi(R, \mu) d\mu. \quad (8)$$

To satisfy the condition specified by Eq. (7b), we see that we have to take $\tilde{A}_j = 0$ in Eq. (6) since the functions $k_n(z)$ diverge at the origin.¹⁶ Thus, the P_N solution for this problem reduces to

$$\psi(r, \mu) = \frac{1}{2} \sum_{n=0}^N (-1)^n (2n+1) P_n(\mu) \times \sum_{j=1}^J \tilde{B}_j \iota_n(r/\xi_j; R/\xi_j) g_n(\xi_j), \quad (9)$$

where to avoid possible overflows in the computational implementation of the solution and to improve the numerical robustness of the method, we have chosen to work with the iota-ratios,

$$\iota_n(x : y) = i_n(x)/i_0(y), \quad x \leq y \text{ and } y > 0, \quad (10)$$

for $n = 0, 1, \dots, N$, rather than with the $\{i_n(x)\}$ functions themselves, and we have rescaled the $\{\tilde{B}_j\}$ coefficients that appear in Eq. (6) so that

$$B_j = \tilde{B}_j i_0(R/\xi_j), \quad (11)$$

for $j = 1, 2, \dots, J$. Clearly, since $i_0(0) = 1$ and $i_n(x) < i_0(x)$ with $i_n(0) = 0$ for $n \geq 1$ (Ref. 16), we have $0 \leq \iota_n(r/\xi_j; R/\xi_j) \leq 1$ for $n = 0, 1, \dots, N$.

As mentioned in the Appendix, a slight modification in the foregoing procedure is required for handling the conservative case $c = 1$. We note that the first few Chandrasekhar polynomials become the following for $c = 1$:

$$g_0(\xi) = 1, \quad (12a)$$

$$g_1(\xi) = 0, \quad (12b)$$

and

$$g_2(\xi) = -\frac{1}{2}. \quad (12c)$$

Considering the recurrence relation given by Eq. (A.7) in the Appendix for $n = 2, 3, \dots, N$, along with the initial values given by Eqs. (12b) and (12c), we can see that $g_{N+1}(\xi)$ is a polynomial of degree $N - 1$ in ξ when $c = 1$. Therefore, in this case, $g_{N+1}(\xi)$ has only $J - 1$ positive zeros that we denote as $\xi_j, j = 2, 3, \dots, J$. The missing solution that corresponds to ξ_1 is replaced by an exact solution of Eq. (1) that is bounded as $r \rightarrow 0$. Such a solution can be easily seen to be a constant, and so Eq. (9) becomes the following for $c = 1$:

$$\psi(r, \mu) = \frac{1}{2}B_1 + \frac{1}{2} \sum_{n=0}^N (-1)^n (2n+1) P_n(\mu) \times \sum_{j=2}^J B_j \iota_n(r/\xi_j : R/\xi_j) g_n(\xi_j) . \quad (13)$$

Now, the incidence condition specified by Eq. (7a) yields, if $c < 1$,

$$\sum_{n=0}^N (2n+1) P_n(\mu) \sum_{j=1}^J B_j \iota_n(R/\xi_j : R/\xi_j) g_n(\xi_j) = 2f(\mu) \quad (14a)$$

and, if $c = 1$,

$$B_1 + \sum_{n=0}^N (2n+1) P_n(\mu) \sum_{j=2}^J B_j \iota_n(R/\xi_j : R/\xi_j) g_n(\xi_j) = 2f(\mu) , \quad (14b)$$

for $\mu \in (0,1]$. We note that the result expressed by Eq. (14b) can also be obtained by letting $\xi_1 \rightarrow \infty$ in Eq. (14a).

Clearly, Eqs. (14a) and (14b) can only be satisfied in an approximate way by the P_N method. In this work, we study three simple ways of generating approximate P_N boundary conditions from Eqs. (14a) and (14b): the shifted-Legendre (SL) projection scheme introduced for plane-geometry problems by Garcia and Siewert¹⁸ and the well-known Marshak¹ and Mark¹⁹ projection schemes.

III.B. Solution Using the SL Projection Scheme

For the SL projection scheme, we multiply Eqs. (14a) and (14b) by $P_\alpha(2\mu - 1)$, for $\alpha = 0, 1, \dots, N$, and integrate the resulting equations over μ from 0 to 1 to obtain, if $c < 1$,

$$\sum_{j=1}^J B_j \sum_{n=\alpha}^N (2n+1) C_{\alpha,n} \iota_n(R/\xi_j : R/\xi_j) g_n(\xi_j) = 2F_\alpha \quad (15a)$$

and, if $c = 1$,

$$B_1 \delta_{\alpha,0} + \sum_{j=2}^J B_j \sum_{n=\alpha}^N (2n+1) C_{\alpha,n} \iota_n(R/\xi_j : R/\xi_j) g_n(\xi_j) = 2F_\alpha , \quad (15b)$$

for $\alpha = 0, 1, \dots, N$. Here, $\delta_{\alpha,0}$ is the Kronecker delta, and we have used the definitions

$$C_{\alpha,n} = \int_0^1 P_\alpha(2\mu - 1) P_n(\mu) d\mu \quad (16)$$

and

$$F_\alpha = \int_0^1 P_\alpha(2\mu - 1) f(\mu) d\mu . \quad (17)$$

We recall that the SL projection scheme generates twice as many equations than unknowns,¹⁸ and so the resulting overdetermined systems of linear algebraic equations that are expressed by Eqs. (15a) and (15b) have to be solved in a least-squares sense for the $\{B_j\}$ coefficients.

Finally, once we have determined the $\{B_j\}$ constants by solving either Eq. (15a) or Eq. (15b), depending on the case, we can immediately find the P_N approximation to the angular flux from either Eq. (9) or Eq. (13). In addition, a P_N approximation to the albedo A^* defined by Eq. (8) can be computed from

$$A_N = 1 - \left[\int_0^1 \mu f(\mu) d\mu \right]^{-1} \sum_{j=j_s}^J B_j \iota_1(R/\xi_j : R/\xi_j) g_1(\xi_j) , \quad (18)$$

where $j_s = 1$ for $c < 1$ and $j_s = 2$ for $c = 1$. For $c = 1$, we know from the physics of the problem that $A^* = 1$, and noting that $g_1(\xi) \equiv 0$, we can see that Eq. (18) yields $A_N = 1$ for all N .

III.C. Solution Using the Marshak Projection Scheme

For the Marshak projection scheme,¹ we multiply Eqs. (14a) and (14b) by $P_{2\alpha-1}(\mu)$, for $\alpha = 1, 2, \dots, J$, and integrate the resulting equations over μ from 0 to 1 to obtain, if $c < 1$,

$$\sum_{j=1}^J B_j \sum_{n=0}^N (2n+1) S_{\alpha,n} \iota_n(R/\xi_j : R/\xi_j) g_n(\xi_j) = 2G_\alpha \quad (19a)$$

and, if $c = 1$,

$$B_1 S_{\alpha,0} + \sum_{j=2}^J B_j \sum_{n=0}^N (2n+1) S_{\alpha,n} \iota_n(R/\xi_j : R/\xi_j) g_n(\xi_j) = 2G_\alpha , \quad (19b)$$

for $\alpha = 1, 2, \dots, J$. Here, we have defined

$$S_{\alpha,n} = \int_0^1 P_{2\alpha-1}(\mu)P_n(\mu)d\mu \quad (20)$$

and

$$G_\alpha = \int_0^1 P_{2\alpha-1}(\mu)f(\mu)d\mu. \quad (21)$$

Equations (19) are systems of J linear algebraic equations to be solved for the J unknowns $\{B_j\}$. Once these coefficients are available, we can find the P_N approximation to the angular flux from either Eq. (9) if $c < 1$ or Eq. (13) if $c = 1$. In addition, as for the SL scheme, a P_N approximation to the albedo A^* can be computed from Eq. (18).

III.D. Solution Using the Mark Projection Scheme

The projection scheme for obtaining the Mark boundary conditions¹⁹ can be formulated by multiplying Eqs. (14a) and (14b) by the Dirac delta distribution $\delta(\mu - \mu_\alpha)$, where μ_α , $\alpha = 1, 2, \dots, J$, are the positive zeros of the Legendre polynomial $P_{N+1}(\mu)$, and integrating the resulting equations over μ from 0 to 1. We get, if $c < 1$,

$$\sum_{j=1}^J B_j \sum_{n=0}^N (2n+1)P_n(\mu_\alpha)\iota_n(R/\xi_j : R/\xi_j)g_n(\xi_j) = 2f(\mu_\alpha) \quad (22a)$$

and, if $c = 1$,

$$B_1 + \sum_{j=2}^J B_j \sum_{n=0}^N (2n+1)P_n(\mu_\alpha)\iota_n(R/\xi_j : R/\xi_j)g_n(\xi_j) = 2f(\mu_\alpha), \quad (22b)$$

for $\alpha = 1, 2, \dots, J$. Equations (22) are systems of J linear algebraic equations to be solved for the J unknowns $\{B_j\}$.

III.E. Computational Methods

We now discuss briefly the computational methods used in our FORTRAN implementation of the solutions developed in Secs. III.B, III.C, and III.D.

With the help of a three-term recurrence relation involving only the even Chandrasekhar polynomials and the closure relation $g_{N+1}(\xi) = 0$, it has been shown²⁰ that the P_N eigenvalues $\{\xi_j\}$ are given by the square roots of the eigenvalues of a special tridiagonal matrix of order J . In this work,

subroutines FIGI and IMTQL1 from EISPACK (Ref. 21) were used for computing the squares of the P_N eigenvalues.

The Chandrasekhar polynomials $\{g_n(\xi_j)\}$ were computed as discussed in Ref. 22 except that the starting ratio for backward recurrence when $\xi_j > 1$ was taken to be $g_{N+1}(\xi_j)/g_N(\xi_j) = 0$. It should be mentioned that the need for solving a linear system when $\xi_j > 1$ does not show up in this work since the problem we are solving here is azimuthally symmetric, and as mentioned in Ref. 22 backward recurrence is sufficient in such a case.

In order to compute the iota-ratios defined by Eq. (10), we have used backward recurrence, which is known to be the stable way of computing the modified spherical Bessel functions of the first kind.³ To describe our procedure, we define

$$\rho_n(x) = \iota_{n+1}(x : y)/\iota_n(x : y) = i_{n+1}(x)/i_n(x), \quad (23)$$

for $n = 0, 1, \dots$, divide the three-term recurrence relation involving $i_{n-1}(x)$, $i_n(x)$, and $i_{n+1}(x)$ by $i_n(x)$, and rearrange the resulting equation to obtain

$$\rho_{n-1}(x) = [(2n+1)/x - \rho_n(x)]^{-1}. \quad (24)$$

We begin the calculation by using Eq. (24) for $n = N + M, N + M - 1, \dots, N + 1$, where $M > 1$ is arbitrary (we used $M = 20$ in our program), with starting value $\rho_{N+M}(x)$ arbitrarily set to zero, and store the value obtained for $\rho_N(x)$. Next, we increase the value of M , repeat the calculation, and compare the value obtained for $\rho_N(x)$ with that of the previous step. We keep increasing M and repeating the calculation until we get convergence in the value of $\rho_N(x)$ to working precision (for example, 16 decimal digits when using DP). Once convergence is achieved, we use Eq. (24) for $n = N, N - 1, \dots, 1$ to compute the remaining rho-ratios. The desired iota-ratios are then given by

$$\iota_0(x : y) = \begin{cases} (y/x)e^{-(y-x)}\left(\frac{1-e^{-2x}}{1-e^{-2y}}\right), & x > 0, \\ \frac{2ye^{-y}}{1-e^{-2y}}, & x = 0, \end{cases} \quad (25a)$$

and

$$\iota_{n+1}(x : y) = \rho_n(x)\iota_n(x : y), \quad (25b)$$

for $n = 0, 1, \dots, N - 1$.

The constants $\{C_{\alpha,n}\}$ and $\{S_{\alpha,n}\}$ defined by Eqs. (16) and (20), respectively, were generated accurately and efficiently with recurrence schemes reported in previous works.^{18,20} In this regard, we note that Eq. (25b) of Ref. 20 should be used only for even values of l , i.e., $l = 0, 2, 4, \dots, N - 3$.

Finally, the linear systems defined by Eqs. (15), (19), and (22) were solved using three different techniques: Gaussian elimination, QR decomposition, and SVD. In the case of the SL projection scheme, the linear system is overdetermined ($N \times J$), and so, to apply Gaussian elimination, we used a least-squares formulation with equal weights that yields a set of J normal equations for the J unknowns.¹⁸ On the other hand, the linear systems obtained from the Marshak and Mark projection schemes are square ($J \times J$), and so Gaussian elimination was applied directly on those systems. Solutions by Gaussian elimination were obtained with subroutines DGECO and DGESL from LINPACK (Ref. 23). Concerning the other more powerful (and more expensive) solution techniques, we note that the least-squares solutions based on the QR decomposition were obtained with subroutine DQRST from LINPACK, while the least-squares solutions based on SVD were obtained with subroutine MINFIT from EISPACK (Ref. 24); another SVD implementation (subroutine DSVDC from LINPACK) was tried with similar results.

III.F. Numerical Results and Discussion

We begin this section by reporting in Tables I, II, and III our numerical results for several orders of the P_N approximation to the albedo, as defined by Eq. (18), for the most difficult case considered in Table I of the work by Aronson³ [$c = 0.9$, $R = 0.5$, $L = 0$, and $f(\mu) = \mu$], and we use that case to compare the performance of the studied projection schemes and linear-equation solvers. The reference results reported in Tables I, II, and III were obtained with the use of SVD in quadruple precision (QP) (approximately 32 decimal digits of precision) and confirmed with QR decomposition, also in QP. These results are thought to be accurate to within ± 1 in the seventh significant figure, except the results for $29 \leq N \leq 199$ in Table III, which may have larger deviations in the seventh figure.

In Table I, which shows the results obtained for the SL projection scheme, we can see that all three ways of solving the linear system—Gaussian elimination on the normal equations (GENE), QR decomposition, and SVD—give at least five significant figures of accuracy in DP,

with the last two ways being slightly more accurate. It should be mentioned that the criterion used to report the number of figures of the double-precision results in all the tables of this work was agreement with the reference results to within ± 2 in the last figure, unless otherwise noted. Also, in this section, the thresholds that have to be given as inputs to the QR and SVD solvers were taken to be equal to the square root of the number of rows times 10^{-14} for double-precision calculations (times 10^{-30} for quadruple-precision calculations).

In Tables II and III, which show the results obtained for the Marshak and Mark projection schemes, respectively, we can see that the Gaussian elimination results in double precision (GE-DP) become inaccurate for $N = 15$. The use of QP does not help much, as the results become inaccurate for $N = 29$. A moderate, but still insufficient, improvement in the accuracy (i.e., from one or no significant figure to three significant figures) was observed when full pivoting routines (LAPACK subroutines DGETC2 and DGESC2) were used. On the other hand, QR-DP and SVD-DP perform better, yielding at least six significant figures in the Marshak scheme and five figures in the Mark scheme.

A general trend that is apparent in Tables I, II, and III is that the GENE-DP, QR-DP, and SVD-DP results become less accurate for intermediate values of N and eventually recover full accuracy as N is increased past $N = 199$. In trying to find an explanation for this numerical behavior, we have observed that the columns that are disregarded in the QR calculations

TABLE I

The Albedo A_N for a Sphere with $c = 0.9$, $R = 0.5$, $L = 0$, and $f(\mu) = \mu$: Results from the SL Projection Scheme

N	GENE-DP	QR-DP	SVD-DP	Reference
1	0.9513281	0.9513281	0.9513281	0.9513281
3	0.9288570	0.9288570	0.9288570	0.9288570
5	0.9288822	0.9288822	0.9288822	0.9288822
7	0.9289371	0.9289371	0.9289371	0.9289371
9	0.92894	0.9289582	0.9289582	0.9289582
11	0.92895	0.9289669	0.9289670	0.9289670
13	0.92896	0.92897	0.92897	0.9289712
15	0.92896	0.92897	0.92897	0.9289733
17	0.92896	0.92897	0.92897	0.9289745
19	0.92896	0.928973	0.92897	0.9289752
29	0.92897	0.92897	0.92897	0.9289757
39	0.92897	0.928974	0.928974	0.9289760
99	0.928975	0.928976	0.928976	0.9289765
199	0.928976	0.9289764	0.928976	0.9289766
399	0.9289765	0.9289766	0.9289766	0.9289767
799	0.9289767	0.9289767	0.9289767	0.9289767

TABLE II

The Albedo A_N for a Sphere with $c = 0.9$, $R = 0.5$, $L = 0$, and $f(\mu) = \mu$: Results from the Marshak Projection Scheme

N	GE-DP	GE-QP	QR-DP	SVD-DP	Reference
1	0.9357939	0.9357939	0.9357939	0.9357939	0.9357939
3	0.9294310	0.9294310	0.9294310	0.9294310	0.9294310
5	0.9290687	0.9290687	0.9290687	0.9290687	0.9290687
7	0.9290061	0.9290061	0.9290061	0.9290061	0.9290061
9	0.9289888	0.9289888	0.9289888	0.9289888	0.9289888
11	0.9289826	0.9289826	0.9289826	0.9289826	0.9289826
13	0.9289	0.9289799	0.928980	0.928980	0.9289799
15	0.92	0.9289786	0.9289787	0.9289787	0.9289786
17	0.9	0.9289779	0.928980	0.928978	0.9289779
19	0.91	0.9289775	0.928978	0.9289777	0.9289775
29	0.9	0.9	0.928976	0.928976	0.9289769
39	0.9	0.9	0.928976	0.928976	0.9289767
99	—	0.928	0.928976	0.928976	0.9289767
199	0.92	0.9	0.9289765	0.9289765	0.9289767
399	0.9	1.0	0.928976	0.9289767	0.9289767
799	1.0	0.927	0.9289767	0.9289768	0.9289768

TABLE III

The Albedo A_N for a Sphere with $c = 0.9$, $R = 0.5$, $L = 0$, and $f(\mu) = \mu$: Results from the Mark Projection Scheme

N	GE-DP	GE-QP	QR-DP	SVD-DP	Reference
1	0.9441557	0.9441557	0.9441557	0.9441557	0.9441557
3	0.9298588	0.9298588	0.9298588	0.9298588	0.9298588
5	0.9291638	0.9291638	0.9291638	0.9291638	0.9291638
7	0.9290391	0.9290391	0.9290391	0.9290391	0.9290391
9	0.9290032	0.9290032	0.9290032	0.9290032	0.9290032
11	0.9289899	0.9289899	0.9289899	0.9289899	0.9289899
13	0.9289	0.9289840	0.92899	0.92899	0.9289840
15	0.927	0.9289811	0.92899	0.92897	0.9289811
17	0.93	0.9289795	0.928978	0.92898	0.9289795
19	0.94	0.9289786	0.928978	0.928978	0.9289786
29	0.9	0.9290	0.92897	0.92897	0.9289774
39	0.92	0.930	0.92898	0.92898	0.9289775
99	0.94	0.9290	0.92898	0.92898	0.9289768
199	0.92	0.93	0.928978	0.928978	0.9289770
399	0.94	0.930	0.928977	0.9289766	0.9289768
799	—	1.0	0.9289767	0.9289769	0.9289768

correspond, preferentially, to the modes related to the P_N eigenvalues ξ_j in the interval $(0, 1)$ that are closest to the end-point one. Noting that for $\xi_j \in (0, 1)$ the argument R/ξ_j

of the modified spherical Bessel functions of the first kind is closest to zero when $\xi_j \rightarrow 1$, we have concluded that the nearly linear dependence of some columns is nothing more

than a manifestation of a loss of information because all of the modified spherical Bessel functions of the first kind (except the first) go to zero when the argument goes to zero. A similar, but less specific, observation in this direction has been given by Sahni and Sharma.²⁵ We believe the reason why the method becomes less accurate for intermediate values of N is that the troublesome modes, which are considered in the GENE-DP calculation and eliminated from the QR and SVD calculations, are relatively more important in that range of N and become less important as N is increased. Finally, considering also other cases that we tried, we have concluded that the Marshak scheme and SVD are the best choices in terms of accuracy for albedo calculations, when using DP.

In Table IV, we show the effect of varying the value of c in Aronson’s most difficult case. We can see that the deviations of the SVD-DP results with respect to those of SVD-QP are slightly larger for low values of c , but we get at least five significant figures of accuracy. The SVD-QP results reported in Table IV are thought to be accurate to within ± 1 in the seventh significant

figure, except the results for $29 \leq N \leq 199$, which may have larger deviations in the last figure.

In Table V, we give an answer to the natural question to be asked at this point: What happens if the radius of the sphere is reduced in Aronson’s most difficult case? We can see in Table V that the SVD-DP implementation of the Marshak scheme yields at least five significant figures of accuracy for values of R as small as 5.0×10^{-4} . To be sure of the good behavior of SVD-DP for cases defined by very small radii, we have reduced R even further (down to 5.0×10^{-9}), with good results.

In Table VI, we tabulate our converged results for the albedo, obtained for different scattering orders (different values of L) in a synthetic kernel²⁶ that is known as the binomial law and is defined by

$$p(\mu_0) = \frac{L+1}{2^L} (1 + \mu_0)^L = \sum_{l=0}^L (2l+1) f_l P_l(\mu_0), \quad (26)$$

TABLE IV

The Albedo A_N for Spheres with $R = 0.5$, $L = 0$, $f(\mu) = \mu$, and Various Values of c : Results from the Marshak Projection Scheme

N	$c = 0.1$		$c = 0.3$		$c = 0.7$	
	SVD-DP	SVD-QP	SVD-DP	SVD-QP	SVD-DP	SVD-QP
1	0.5536237	0.5536237	0.6319142	0.6319142	0.8206124	0.8206124
3	0.5221872	0.5221872	0.6039630	0.6039630	0.8044680	0.8044680
5	0.5198695	0.5198695	0.6020075	0.6020075	0.8034743	0.8034743
7	0.5194562	0.5194562	0.6016627	0.6016627	0.8033019	0.8033019
9	0.5193428	0.5193428	0.6015681	0.6015681	0.8032544	0.8032544
11	0.519303	0.5193022	0.601534	0.6015342	0.8032376	0.8032374
13	0.51929	0.5192849	0.601522	0.6015198	0.803231	0.8032301
15	0.519278	0.5192766	0.601514	0.6015128	0.803227	0.8032266
17	0.519270	0.5192722	0.601508	0.6015091	0.803224	0.8032247
19	0.519268	0.5192697	0.601506	0.6015070	0.803222	0.8032236
29	0.51926	0.5192657	0.60150	0.6015036	0.80322	0.8032219
39	0.51926	0.5192646	0.60150	0.6015027	0.803219	0.8032214
99	0.519262	0.5192642	0.601501	0.6015024	0.803220	0.8032213
199	0.519264	0.5192645	0.601502	0.6015026	0.803221	0.8032214
399	0.5192645	0.5192647	0.6015026	0.6015028	0.8032214	0.8032215
799	0.5192648	0.5192649	0.6015029	0.6015029	0.8032215	0.8032216

TABLE V

The Albedo A_N for Spheres of Very Small Radii with $c = 0.1$, $L = 0$, and $f(\mu) = \mu$: Results from the Marshak Projection Scheme

N	$R = 0.05$		$R = 0.005$		$R = 0.0005$	
	SVD-DP	SVD-QP	SVD-DP	SVD-QP	SVD-DP	SVD-QP
1	0.9417730	0.9417730	0.9940180	0.9940180	0.9994002	0.9994002
3	0.9351881	0.9351881	0.9933044	0.9933044	0.9993282	0.9993282
5	0.9349381	0.9349381	0.9932798	0.9932799	0.9993257	0.9993258
7	0.9348992	0.9348992	0.9932761	0.9932760	0.999325	0.9993254
9	0.934890	0.9348889	0.993274	0.9932750	0.999324	0.9993253
11	0.934884	0.9348853	0.993273	0.9932747	0.999324	0.9993253
13	0.93488	0.9348837	0.993273	0.9932745	0.999324	0.9993252
15	0.93488	0.9348831	0.993272	0.9932743	0.999324	0.9993252
17	0.93488	0.9348826	0.993272	0.9932742	0.999324	0.9993252
19	0.93487	0.9348822	0.993272	0.9932741	0.999324	0.9993252
29	0.93488	0.9348816	0.99327	0.9932742	0.999325	0.9993252
39	0.93488	0.9348813	0.99327	0.9932741	0.999325	0.9993252
99	0.934879	0.9348813	0.993273	0.9932742	0.999325	0.9993252
199	0.934881	0.9348815	0.993273	0.9932742	0.999325	0.9993252
399	0.934881	0.9348817	0.993274	0.9932742	0.999325	0.9993252
799	0.934881	0.9348818	0.993274	0.9932743	0.9993251	0.9993252

TABLE VI

The Albedo A_N of a Sphere with $c = 0.9$ and $f(\mu) = \mu$ for Various Values of R and L : Converged Results from the Marshak Projection Scheme and SVD-DP

L	$R = 0.5$	$R = 1.0$	$R = 2.0$	$R = 5.0$	$R = 10.0$
0	0.928976774	0.865988724	0.763665725	0.601315927	0.525253388
19	0.928166035	0.862329721	0.746796144	0.501712998	0.300160401
49	0.928028748	0.861796323	0.744777309	0.490944641	0.269136825
99	0.927975803	0.861588216	0.743977756	0.486654546	0.256728392
199	0.927947713	0.861477183	0.743547352	0.484312916	0.249903725
299	0.927938088	0.861439040	0.743398831	0.483497603	0.247507970
399	0.927933225	0.861419745	0.743323570	0.483082848	0.246283733

where the Legendre coefficients $\{f_l\}$ can be computed exactly by recurrence with $f_0 = 1$ and²⁷

$$f_l = \left(\frac{L+1-l}{L+1+l} \right) f_{l-1}, \tag{27}$$

for $l = 1, 2, \dots, L$. Note that for $l > L$ all $f_l = 0$. The binomial law describes scattering that becomes more and more pronounced in the forward direction as L is increased. Indeed, it is easy to see that Eq. (26) reduces to $p(\mu_0) = \delta(\mu_0 - 1)$ in the limit of $L \rightarrow \infty$. The results reported in Table VI are thought to be accurate in all figures shown and were obtained with N between 9999 and 12999 (depending on the case) in the SVD-DP implementation of the Marshak projection scheme.

To close this section, we report in Table VII our converged results, from the SVD-DP implementation of the Mark projection scheme, for the scalar flux and current for different scattering orders in the binomial law. The Mark projection scheme was found to converge faster than the Marshak projection scheme for these quantities. The results in Table VII are thought to be accurate to within ± 1 in the last significant figure and were obtained with N between 5999 and 8999.

IV. THE CRITICAL-SPHERE PROBLEM

We consider in this section the problem of finding the critical radius of a sphere. We assume isotropic fission

TABLE VII

The Scalar Flux $\phi_0(r)$ and the Current $\phi_1(r)$ for a Sphere with $c = 0.9$, $R = 0.5$, and $f(\mu) = \mu$: Converged Results from the Mark Projection Scheme and SVD-DP

r/R	$L = 0$		$L = 19$		$L = 399$	
	$\phi_0(r)$	$-\phi_1(r)$	$\phi_0(r)$	$-\phi_1(r)$	$\phi_0(r)$	$-\phi_1(r)$
0.0	1.7875	0.0	1.8760	0.0	1.9010	0.0
0.1	1.7831	2.9748(-3) ^a	1.8703	3.1210(-3)	1.8950	3.1623(-3)
0.2	1.7700	5.9234(-3)	1.8531	6.2077(-3)	1.8768	6.2884(-3)
0.3	1.7476	8.8186(-3)	1.8240	9.2248(-3)	1.8459	9.3407(-3)
0.4	1.7148	1.1630(-2)	1.7819	1.2134(-2)	1.8014	1.2279(-2)
0.5	1.6700	1.4323(-2)	1.7253	1.4894(-2)	1.7417	1.5060(-2)
0.6	1.6106	1.6856(-2)	1.6519	1.7454(-2)	1.6645	1.7630(-2)
0.7	1.5324	1.9171(-2)	1.5576	1.9753(-2)	1.5658	1.9927(-2)
0.8	1.4272	2.1192(-2)	1.4354	2.1710(-2)	1.4384	2.1868(-2)
0.9	1.2770	2.2792(-2)	1.2689	2.3198(-2)	1.2663	2.3323(-2)
1.0	9.8661(-1)	2.3674(-2)	9.7401(-1)	2.3945(-2)	9.6832(-1)	2.4022(-2)

^aRead as 2.9748×10^{-3} .

TABLE VIII

The Critical Radius for the Case $c = 2.0$ and $L = 0$

N	SL Projection Scheme		Marshak Projection Scheme	
	SVD-DP	SVD-QP	SVD-DP	SVD-QP
1	1.0956395	1.0956395	1.0956395	1.0956395
3	0.9823991	0.9823991	0.9911102	0.9911102
5	0.9868723	0.9868723	0.9908852	0.9908852
7	0.9902374	0.9902374	0.9907076	0.9907076
9	0.9906254	0.9906254	0.9906510	0.9906510
11	0.9906029	0.9906029	0.9906286	0.9906286
13	0.990603	0.9906042	0.990620	0.9906184
15	0.99060	0.9906047	0.990615	0.9906132
17	0.99060	0.9906051	0.990611	0.9906104
19	0.990605	0.9906052	0.990610	0.9906088
29	0.990605	0.9906055	0.9906063	0.9906063
39	0.990605	0.9906055	0.9906056	0.9906058
99	0.9906055	0.9906056	0.9906054	0.9906056
199	0.9906056	0.9906056	0.9906055	0.9906056
399	0.9906056	0.9906056	0.9906056	0.9906056
799	0.9906056	0.9906056	0.9906056	0.9906056

and anisotropic scattering, and so, we take the parameter c in Eq. (1) to be known and given by

$$c = \frac{v\sigma_f + \sigma_s}{\sigma} > 1, \tag{28}$$

where σ_f , σ_s , σ are, respectively, the fission, scattering, and total cross sections and v is the mean number of neutrons emitted per fission event. We note that to take

into account scattering anisotropy in the presence of isotropic fission, the Legendre coefficients $\{f_l\}$ of the scattering law must be multiplied by c_s/c , where $c_s = \sigma_s/\sigma$, for $l \geq 1$, prior to being used in Eq. (1).

IV.A. Formulation

The problem is formulated by Eq. (1) subject to

$$\psi(R, -\mu) = 0, \quad (29a)$$

for $\mu \in (0,1]$, and

$$\lim_{r \rightarrow 0} \psi(r, \mu) < \infty, \quad (29b)$$

for $\mu \in [-1,1]$. We look for the (smallest) value of the critical radius R that is associated with a physically meaningful solution of Eqs. (1) and (29) (i.e., a positive angular flux everywhere in the sphere).

Since in all the cases studied in this work we have encountered only one pair of purely imaginary P_N eigenvalues, denoted here by $\pm \xi_1 = \pm i\eta$, where η is real and positive, we find we can modify slightly the P_N solution developed in Sec. III to write our P_N solution of Eq. (1) that satisfies Eq. (29b) in terms of real quantities only. We find that Eq. (9) becomes

$$\begin{aligned} \psi(r, \mu) = & \frac{1}{2} \sum_{n=0}^N (-1)^n (2n+1) P_n(\mu) \\ & \times \left[B_1 j_n(r/\eta) f_n(\eta) + \sum_{j=2}^J B_j t_n(r/\xi_j : R/\xi_j) g_n(\xi_j) \right], \end{aligned} \quad (30)$$

where

$$j_n(x) = \sqrt{\frac{\pi}{2x}} J_{n+1/2}(x) \quad (31)$$

is the spherical Bessel function of the first kind¹⁶ that satisfies the three-term recurrence relation

$$j_{n-1}(x) + j_{n+1}(x) = \frac{2n+1}{x} j_n(x), \quad (32)$$

for $n = 1, 2, \dots$, with initial values

$$j_0(x) = \frac{\sin x}{x} \quad (33a)$$

and

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}. \quad (33b)$$

In addition, the polynomials $\{f_n(\eta)\}$ are related to the Chandrasekhar polynomials by $f_n(\eta) = (-i)^n g_n(i\eta)$ and satisfy

$$(n+1)f_{n+1}(\eta) - nf_{n-1}(\eta) = h_n \eta f_n(\eta), \quad (34)$$

for $n = 0, 1, \dots$, with

$$f_0(\eta) = 1. \quad (35)$$

For this problem, we use the Marshak and SL projection schemes for generating approximate P_N boundary conditions from Eq. (29a). Moreover, as we intend to allow the use of least-squares solutions for which the number of equations considered is, in general, not equal to the number of unknowns, we avoid the usual procedure of searching the critical radius that is based on finding a zero of a determinant.⁴

IV.B. Solution Using the Marshak Projection Scheme

Following the procedure discussed in Sec. III.C and choosing the arbitrary normalization $B_1 = 1$, which we are allowed to do, since for this problem any multiple of a solution is also a solution, we find that R and the unknown coefficients B_j , $j = 2, 3, \dots, J$, must satisfy the equation

$$\begin{aligned} \sum_{j=2}^J B_j \sum_{n=0}^N (2n+1) S_{\alpha,n} t_n(R/\xi_j : R/\xi_j) g_n(\xi_j) \\ = - \sum_{n=0}^N (2n+1) S_{\alpha,n} j_n(R/\eta) f_n(\eta), \end{aligned} \quad (36)$$

for $\alpha = 1, 2, \dots, J$. In the P_1 approximation, we have only one equation, namely,

$$\frac{1}{2} j_0(R/\eta) + j_1(R/\eta) f_1(\eta) = 0, \quad (37)$$

where $\eta = |(h_0 h_1)^{-1/2}|$. Using the explicit representations of the spherical Bessel functions and $f_1(\eta)$, we get from Eq. (37)

$$(R + 2h_0 \eta^2) \sin(R/\eta) - 2h_0 \eta R \cos(R/\eta) = 0. \quad (38)$$

To solve Eq. (38) for R , we use Newton's method with a starting value chosen as discussed in Sec. IV.D.

For $N \geq 3$, in order to avoid having to evaluate derivatives exactly, which becomes cumbersome as N is increased, we use the regula-falsi technique. This requires two initial estimates of the critical radius, say $R^{(1)}$ and $R^{(2)}$ (see our choices in Sec. IV.D). First, we solve, in a least-squares sense, the linear system that is obtained from Eq.

(36) for $\alpha = 2, 3, \dots, J$, once with $R^{(1)}$ replacing R and again with $R^{(2)}$ replacing R . This yields the initial estimates $B_j^{(1)}$ and $B_j^{(2)}$, $j = 2, 3, \dots, J$. Next, we apply regula falsi to Eq. (36) for $\alpha = 1$ to determine an updated estimate of the critical radius $R^{(3)}$. Then, we continue this iterative process, solving the last $J - 1$ equations of Eq. (36) in alternation with Eq. (36) for $\alpha = 1$, until two consecutive estimates of the critical radius R and the coefficients B_j , $j = 2, 3, \dots, J$, do not differ by more than a prescribed tolerance.

IV.C. Solution Using the SL Projection Scheme

Using the SL projection scheme discussed in Sec. III.B and the normalization $B_1 = 1$ introduced for the Marshak scheme, we find that we have to solve, in a least-squares sense, the $N + 1$ equations obtained by taking $\alpha = 0, 1, 2, \dots, N$ in

$$\sum_{j=2}^J B_j \sum_{n=\alpha}^N (2n + 1) C_{\alpha,n} t_n(R/\xi_j : R/\xi_j) g_n(\xi_j) = - \sum_{n=\alpha}^N (2n + 1) C_{\alpha,n} j_n(R/\eta) f_n(\eta), \quad (39)$$

for J unknowns that are the critical radius R and the coefficients B_j , $j = 2, 3, \dots, J$. To do that, we follow an approach that is similar to the iterative procedure just discussed for the Marshak scheme and gives results identical to those of the Marshak scheme when $N = 1$. The only difference between the procedures is that here we use an equation that is obtained by adding the two forms of Eq. (39) for $\alpha = 1$ and $\alpha = 2$ to update the estimates of the critical radius and a least-squares solution of the last $N - 1$ equations of Eq. (39) to find and update estimates of B_j , $j = 2, 3, \dots, J$.

IV.D. Computational Methods

Most of the computational methods used for solving the critical-sphere problem have already been discussed in Sec. III.E. The only new aspects that we need to discuss here are (1) the procedure we use for computing the P_N eigenvalues when $c > 1$, (2) the calculation of the spherical Bessel functions of the first kind $\{j_n(x)\}$ and the polynomials $\{f_n(\eta)\}$ defined by Eqs. (34) and (35), and (3) the selection of initial estimates for the critical radius that are required by the iterative procedures discussed in Secs. IV.B and IV.C.

With regard to the P_N eigenvalues, we note that they can still be obtained from the squares of the eigenvalues

of a tridiagonal matrix when $c > 1$. Unfortunately, as that matrix cannot be reduced to a form that allows the application of the EISPACK routines for finding the eigenvalues of a special tridiagonal matrix that are mentioned in Sec. III.E, the best we could do here was to use a routine developed for finding the eigenvalues of Hessenberg matrices (we used EISPACK subroutine HQR).

The functions $\{j_n(x)\}$ are computed by backward recurrence using the ratios $j_{n+1}(x)/j_n(x)$, $n = 0, 1, \dots, N - 1$, in pretty much the same way as described for the iota-ratios in Sec. III.E. The polynomials $\{f_n(\eta)\}$ are also computed by backward recurrence, as done for the Chandrasekhar polynomials $\{g_n(\xi_j)\}$ when ξ_j is real and > 1 . Indeed, it can be seen that the recurrence relation of $\{f_n(\eta)\}$ differs only by a sign from that of the Chandrasekhar polynomials.

The initial estimate of the critical radius for the P_1 equation that is solved by Newton's method for both the Marshak and SL projection schemes [Eq. (38)] is taken from the end-point method in spherical geometry, which is very accurate for isotropic scattering.²⁸ The end-point result can be written as

$$R^{(0)} = \pi|v_0| - x_0, \quad (40)$$

where v_0 is the discrete eigenvalue for isotropic scattering and x_0 is the extrapolation distance.²⁸ We used the unnumbered equation on the top of p. 95 of Ref. 28 to obtain an approximate value of x_0 and the expansions for $1/|v_0|^2$ given by Eqs. (74) and (77) of Ref. 29 to obtain an approximate value of $|v_0|$. We note that the break point to switch from one of the expansions of Ref. 29 to the other was taken to be $c = 1.5$.

As mentioned before, for $N \geq 3$ our iterative procedure is based on the regula-falsi technique, which requires two initial estimates of the parameter being sought. For that purpose, we first find a single initial value $R^{(0)}$, as described next, and then multiply it by $(1 \pm \epsilon)$, with ϵ set arbitrarily to 0.02, to obtain the required initial values $R^{(1)}$ and $R^{(2)}$. Regarding our choice of $R^{(0)}$, we have used the result of the P_1 approximation when $N = 3$ and the result of the P_3 approximation when $N > 3$.

We note that the careful procedure of selecting good initial values for the regula-falsi technique just described turned out to be very important in high order. A good selection of initial values is crucial for high-order calculations because one needs to isolate the desired fundamental mode from the higher harmonics, which is something that becomes progressively more difficult as

the order of approximation is increased. For low and moderate values of N , a less elaborate procedure could be used.

IV.E. Numerical Results and Discussion

First, to give an idea of the convergence behavior of the P_N method discussed in Secs. IV.A, IV.B, and IV.C, we list in Table VIII our numerical results for the critical radius, obtained from several orders of the approximation, for the most difficult case considered in Table II of Ref. 4 ($c = 2.0$ and $L = 0$). As SVD was found to perform better than QR decomposition, we give only the SVD results in Table VIII. We can see that the double-precision results deteriorate slightly between $N = 13$ and $N = 39$ for the SL scheme and between $N = 13$ and $N = 19$ for the Marshak scheme, but the SL scheme yields at least five significant figures of accuracy and the Marshak scheme six. The threshold below which a singular value was not considered in the SVD solution was taken to be equal to the square root of the number of rows in the linear system to be solved times 10^{-8} for double-precision calculations (times 10^{-24} for quadruple-precision calculations).

Next, in Tables IX and X, we report, for two values of c_s and various values of c and L , the scattering order of the binomial law, our converged critical-radius results. It is possible to note the strong influence of the degree of scattering anisotropy on the results, especially when more scattering is present relative to absorption and the radius of the sphere is large. For most entries, the converged results were obtained with N between 1999 and 9999 in the SVD-DP implementation of the Marshak scheme; only in the case of nine entries, larger values of N (up to 17999) were required. The column corresponding to $L = 0$ was omitted from

Table X because it repeats that of Table IX. The results in Tables IX and X are thought to be correct in all figures shown, as we have checked them using SVD-QP. Moreover, our $L = 0$ results were found to be in very good agreement with the highly accurate results reported by Kaper et al.³⁰ in Table V of their work. We note that the results of Kaper et al. were generated using the method of singular eigenfunctions to solve the pseudo problem that is obtained for the case of isotropic scattering. Using our SVD-QP implementation of the Marshak scheme, we have been able to verify that all but one of the entries reported in Table V of Ref. 30 (between 9 and 12 significant figures reported, depending on the value of c) are off by between one and three units in the last figure.

To close this section, we report in Table XI our converged numerical results for the normalized scalar flux $\phi_0(r)/\phi_0(0)$ for three values of c , $c_s = 0.9$, and two values of L . These results were obtained by varying the value of N in our SVD-DP implementation of the Marshak scheme until convergence in the number of figures shown was attained. For $c = 1.01$, $N = 199$ was sufficient for all entries, except the entry corresponding to $r/R = 1.0$ for which $N = 13999$ was needed. For $c = 1.2$ and $L = 0$, $N = 14999$ was required, while for $c = 1.2$ and $L = 399$, we had to use $N = 17999$. Finally, for $c = 1.4$, we had to use $N = 26999$. We conjecture that the increasing difficulty in getting accurate results for the scalar flux as c is increased (or, equivalently, the critical radius of the sphere is decreased) is related to the essence of the P_N method, i.e., the separability hypothesis between the spatial and angular variables in the angular flux representation. Nevertheless, as discussed in Sec. V, we believe it is possible to improve on this aspect of the method.

TABLE IX

The Critical Radius for $c_s = 0.3$ and Different Values of c and L : Converged Results from the Marshak Projection Scheme and SVD-DP

c	$L = 0$	$L = 49$	$L = 99$	$L = 199$	$L = 399$
1.01	17.362440470	20.396242468	20.474600725	20.514725932	20.535040874
1.02	12.027532098	14.065071820	14.116862288	14.143354976	14.156759631
1.05	7.277181794	8.424992160	8.452958389	8.467216067	8.474415070
1.1	4.872714266	5.572409108	5.588497121	5.596662607	5.600774896
1.2	3.172072513	3.564019638	3.572288300	3.576462015	3.578557753
1.3	2.424824980	2.689496214	2.694744711	2.697385444	2.698709240
1.4	1.985343432	2.179940232	2.183621390	2.185469612	2.186395139
1.6	1.476098589	1.596679783	1.598811318	1.599878702	1.600412517
2.0	0.990605572	1.051584313	1.052578201	1.053074592	1.053322526

TABLE X

The Critical Radius for $c_s = 0.9$ and Different Values of c and L : Converged Results from the Marshak Projection Scheme and SVD-DP

c	$L = 19$	$L = 49$	$L = 99$	$L = 199$	$L = 399$
1.01	37.728852673	43.185447607	45.702646319	47.146588427	47.919799122
1.02	25.276334501	28.572542033	30.035061386	30.851366601	31.280168625
1.05	14.226720972	15.677277370	16.268115163	16.581336010	16.741067221
1.1	8.759863096	9.411558791	9.655710731	9.780575937	9.843299585
1.2	5.108330711	5.350156840	5.434640186	5.477004665	5.498151744
1.3	3.632317569	3.757094935	3.799586010	3.820786070	3.831354403
1.4	2.822896882	2.898713101	2.924228888	2.936935146	2.943266471
1.6	1.955075744	1.991514546	2.003653500	2.009689959	2.012697021
2.0	1.211823579	1.225795643	1.230420180	1.232718247	1.233862940

TABLE XI

The Normalized Scalar Flux for a Critical Sphere with $c_s = 0.9$ and Different Values of c and L : Converged Results from the Marshak Projection Scheme and SVD-DP

r/R	$c = 1.01$		$c = 1.2$		$c = 1.4$	
	$L = 0$	$L = 399$	$L = 0$	$L = 399$	$L = 0$	$L = 399$
0.0	1.0	1.0	1.0	1.0	1.0	1.0
0.1	0.9848758	0.9871904	0.988320	0.991697	0.9895	0.9922
0.2	0.9403251	0.9493494	0.953763	0.967010	0.9583	0.9691
0.3	0.8687610	0.8882073	0.897749	0.926589	0.9077	0.9311
0.4	0.7740316	0.8065393	0.822561	0.871484	0.8394	0.8792
0.5	0.6611729	0.7080054	0.731215	0.803084	0.7557	0.8145
0.6	0.5360866	0.5969328	0.627282	0.723020	0.6596	0.7385
0.7	0.4051659	0.4780297	0.514635	0.633013	0.5542	0.6526
0.8	0.2748827	0.3559678	0.397049	0.534527	0.4422	0.5579
0.9	0.1512516	0.2344160	0.277151	0.427700	0.3254	0.4543
1.0	0.0328262	0.1039008	0.144626	0.299213	0.1922	0.3282

V. CONCLUDING REMARKS

A version of the P_N method for spheres that is numerically stable in high order is reported in this work. Having been able to go as high as tens of thousands in the order of the approximation with excellent results, we believe that the use of the method is limited only by the amount of computational resources available.

From all the linear equation solvers and projection schemes of boundary conditions that we tried, we concluded that the combination of SVD and Marshak boundary conditions is the best choice for computing global quantities like the albedo and the critical radius. In addition, we have found that the Mark boundary conditions converge more rapidly than the Marshak boundary conditions for the scalar flux and current in the case of the albedo problem. Furthermore, we have observed that the

number of columns used by SVD when N is large is usually a very small fraction of the total number of columns. This leads to the immediate question: Why does SVD allow us to get greater accuracy by taking more equations and at the same time eliminating more columns as we increase the order of approximation? A possible explanation is that the improvement observed as N is increased comes from the fact that the boundary condition is better represented as we add more equations (rows). And SVD lets us select the modes (columns) that really matter, eliminating those that are linearly dependent (or almost linearly dependent). A similar comment could be made with respect to the QR decomposition.

In our continuing work on this topic, we plan to extend the method to the case of a spherical shell. In addition to the importance of such a problem per se, this will allow the treatment of multilayer spheres in a more

efficient way, by solving for a layer at a time and sweeping across the layers iteratively for convergence.

Finally, we would like to comment on the finding that the convergence rate of the P_N method for pointwise quantities of interest such as the scalar flux and the current is relatively slow (especially at the end points of the spatial interval for large spheres and everywhere for small spheres) when compared to that of the global quantities. In our future work we plan to investigate possible ways of postprocessing our solution to obtain improved results for pointwise quantities with reduced orders of the approximation. If successful, we believe this will be a very useful addition to the method for dealing better with spheres of small radii.

APPENDIX

SOLUTION OF THE MOMENT EQUATIONS

In the manner of Davison,² we try solutions for Eq. (3) in the form

$$\phi_n(r) = F_n(r/\xi)g_n(\xi), \quad (\text{A.1})$$

where ξ is a parameter, to find

$$\begin{aligned} (n+1) \left[\frac{d}{d(r/\xi)} F_{n+1}(r/\xi) + \frac{\xi}{r} (n+2) F_{n+1}(r/\xi) \right] g_{n+1}(\xi) \\ + n \left[\frac{d}{d(r/\xi)} F_{n-1}(r/\xi) - \frac{\xi}{r} (n-1) F_{n-1}(r/\xi) \right] g_{n-1}(\xi) \\ + h_n \xi F_n(r/\xi) g_n(\xi) = 0 \end{aligned} \quad (\text{A.2})$$

for $n = 0, 1, \dots, N$. Now, since the modified spherical Bessel functions of the first kind¹⁶

$$i_n(z) = \sqrt{\frac{\pi}{2z}} J_{n+1/2}(z) \quad (\text{A.3})$$

and of the second kind

$$i_{-n}(z) = \sqrt{\frac{\pi}{2z}} I_{-n-1/2}(z), \quad (\text{A.4})$$

for $n = 0, 1, \dots$, satisfy

$$\frac{d}{dz} f_n(z) + \frac{n+1}{z} f_n(z) = f_{n-1}(z) \quad (\text{A.5a})$$

and

$$\frac{d}{dz} f_n(z) - \frac{n}{z} f_n(z) = f_{n+1}(z), \quad (\text{A.5b})$$

we see at once that if we take either

$$F_n(r/\xi) = (-1)^n i_n(r/\xi) \quad (\text{A.6a})$$

or

$$F_n(r/\xi) = (-1)^n i_{-n}(r/\xi) \quad (\text{A.6b})$$

the terms in brackets in Eq. (A.2) reduce to $-F_n(r/\xi)$. We thus conclude that for Eq. (A.2) to be satisfied, we must have

$$(n+1)g_{n+1}(\xi) + ng_{n-1}(\xi) = h_n \xi g_n(\xi). \quad (\text{A.7})$$

This recurrence relation tells us that $\{g_n(\xi)\}$ is the set of Chandrasekhar polynomials encountered in the P_N solution of the one-speed transport equation in plane geometry. The reason why the same family of polynomials appears both in planar and spherical geometry has been thoroughly discussed by Davison.² The first few Chandrasekhar polynomials are

$$g_0(\xi) = 1, \quad (\text{A.8a})$$

$$g_1(\xi) = h_0 \xi, \quad (\text{A.8b})$$

and

$$g_2(\xi) = \frac{1}{2} (h_0 h_1 \xi^2 - 1). \quad (\text{A.8c})$$

In summary, we conclude that $(-1)^n i_n(r/\xi)g_n(\xi)$ and $(-1)^n i_{-n}(r/\xi)g_n(\xi)$ are solutions to Eq. (3). However, our job is not complete yet since we still need to find the permissible values of the parameter ξ . For this purpose, we use the standard P_N closure $\phi_{N+1}(r) = 0$, which yields the zeros of $g_{N+1}(\xi)$ as the values of ξ that we seek.

Since $N+1$ is even and the Chandrasekhar polynomials of even order have only even powers of the argument (with the highest power being equal to the order) in their explicit expressions,³¹ the zeros of $g_{N+1}(\xi)$ appear as positive/negative pairs that we denote as $\pm \xi_j$, $j = 1, 2, \dots, J = (N+1)/2$. Note that for $c < 1$ all zeros of $g_{N+1}(\xi)$ are real, and we take ξ_j to be positive. For $c = 1$, one pair of zeros ($\pm \xi_1$) becomes unbounded, and a slight modification in the procedure is required, as done for plane geometry;³² the other zeros are real ($\pm \xi_j$, with $\xi_j > 0$, for

$j = 2, 3, \dots, J$). For $c > 1$, at least one pair of zeros must be purely imaginary, and even complex zeros may exist;³³ in this work, we consider only the most relevant case for fission-reactor technology, where just one pair of purely imaginary zeros ($\pm \xi_1$, with $\Im\{\xi_1\} > 0$) exists and the other zeros are real ($\pm \xi_j$, with $\xi_j > 0$, for $j = 2, 3, \dots, J$). The modifications needed to treat other cases are simple.

By superposition, we can write an explicit expression for the $\phi_n(r)$ moment as

$$\begin{aligned} \phi_n(r) = & (-1)^n \sum_{j=1}^J \left[A_j^+ i_{-n}(r/\xi_j) + B_j^+ i_n(r/\xi_j) \right] g_n(\xi_j) \\ & + (-1)^n \sum_{j=1}^J \left[A_j^- i_{-n}(-r/\xi_j) + B_j^- i_n(-r/\xi_j) \right] g_n(-\xi_j), \end{aligned} \tag{A.9}$$

where the coefficients A_j^+ , A_j^- , B_j^+ , and B_j^- for $j = 1, 2, \dots, J$ are to be determined.

Using the symmetry relations

$$g_n(-\xi) = (-1)^n g_n(\xi) \tag{A.10}$$

and (see formulas 10.2.5 and 10.2.6 of Ref. 16)

$$i_n(-z) = (-1)^n i_n(z) \tag{A.11a}$$

and

$$i_{-n}(-z) = (-1)^{n+1} i_{-n}(z), \tag{A.11b}$$

and defining

$$\widehat{A}_j = A_j^+ - A_j^- \tag{A.12a}$$

and

$$\widehat{B}_j = B_j^+ + B_j^-, \tag{A.12b}$$

we find that we can rewrite Eq. (A.9) as

$$\phi_n(r) = (-1)^n \sum_{j=1}^J \left[\widehat{A}_j i_{-n}(r/\xi_j) + \widehat{B}_j i_n(r/\xi_j) \right] g_n(\xi_j). \tag{A.13}$$

We note that Eq. (A.13) is a valid general solution of Eq. (3). However, it has the disadvantage that both of the $i_{-n}(r/\xi_j)$ and $i_n(r/\xi_j)$ functions diverge as $r \rightarrow \infty$. We can have a general solution written in a more convenient way by taking

$$\widehat{A}_j = \frac{\pi}{2} \widetilde{A}_j \tag{A.14a}$$

and

$$\widehat{B}_j = \widetilde{B}_j - \frac{\pi}{2} \widetilde{A}_j \tag{A.14b}$$

in Eq. (A.13). We find

$$\phi_n(r) = \sum_{j=1}^J \left[\widetilde{A}_j k_n(r/\xi_j) + (-1)^n \widetilde{B}_j i_n(r/\xi_j) \right] g_n(\xi_j), \tag{A.15}$$

where $k_n(z)$ denotes the modified spherical Bessel function of the third kind¹⁶

$$\begin{aligned} k_n(z) &= \sqrt{\frac{\pi}{2z}} K_{n+1/2}(z) \\ &= (-1)^{n+1} \frac{\pi}{2} [i_n(z) - i_{-n}(z)]. \end{aligned} \tag{A.16}$$

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