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Calculation of the Asymptotic Diffusion Lengths for Highly Anisotropic Particle Transport*

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A method for calculating the asymptotic diffusion lengths (the so-called discrete eigenvalues) without use of the usual Legendre expansions is presented for the case of one speed particle transport in a highly anisotropically scattering medium. This technique which uses the scattering or phase function directly reduces the problem to a matrix eigenvalue problem. Very accurate numerical results are obtained for low absorption cases (large eigenvalues) and highly forward anisotropic scattering—situations common to radiative transfer problems.

1. INTRODUCTION

The discrete eigenvalues or diffusion lengths in one speed particle transport theory play a dominant role in the description of the asymptotic behavior of the particle density far from sources. Techniques for computing these eigenvalues for anisotropic scattering situations have been investigated by a number of authors [1–4]. In all these investigations, the scattering or phase function was expanded in terms of Legendre polynomials, and while such an expansion has significant analytical advantages, the discrete eigenvalues are found from the zeros of a *dispersion function* which becomes numerically difficult to evaluate for high degrees of anisotropy (or order of the scattering function expansion). Several equivalent forms of the dispersion function have been used but essentially they are of two principle types: integral formulations [1, 5, 6] in which the integrands oscillate rapidly for high order expansions, and formulations involving only polynomials and associated Legendre functions [3, 7] which likewise are difficult to evaluate numerically for very high order expansions.

In this paper a direct technique for evaluating the discrete eigenvalues is presented which does not require the usual Legendre expansions and thereby avoids the numerical problems when very high order expansions (>50) are indicated. Use

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of numerical quadrature in the statement of the eigenvalue problem, immediately reduces the problem to that of the matrix eigenvalue problem encountered in the discrete ordinate formulation of the transport equation [8]. It is shown that this matrix eigenvalue problem can be reduced to a smaller equivalent matrix problem by using the symmetry of Gauss quadrature ordinates and the positive–negative property of the discrete eigenvalues. The reduced matrix eigenvalue problem is found to be well suited for numerical solution by standard techniques, and except for those discrete eigenvalues whose absolute value is very close to unity, this technique produces very accurate results even if the scattering is highly anisotropic.

2. Derivation of the Matrix Eigenvalue Problem

The eigenvalue problem associated with the one speed transport of particles in a medium with plane geometry can be written as [1]

$$\mu^{-1}\left\{\phi_\nu(\mu) - \frac{c}{2}\int_{-1}^{1} d\mu' f(\mu, \mu')\,\phi_\nu(\mu')\right\} = \nu^{-1}\phi_\nu(\mu), \mu \in [-1, 1] \tag{2.1}$$

where c is the mean number of secondary particles produced per collision, ϕ_ν and ν the eigenfunction and eigenvalue respectively (with $\phi_\nu \in L_2[-1, 1]$ and ν complex $\notin[-1, 1]$), and f the azimuthally averaged scattering function

$$f(\mu, \mu') = \frac{1}{2\pi}\int_0^{2\pi} d\phi' f(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') \tag{2.2}$$

where $\boldsymbol{\Omega}'$ and $\boldsymbol{\Omega}$ are, respectively, the unit vectors in the direction of the particle before and after a collision, $\boldsymbol{\Omega} \equiv (\cos^{-1}\mu, \phi)$, $\boldsymbol{\Omega}' \equiv (\cos^{-1}\mu', \phi')$. By using an even N point Gaussian quadrature, Eq. (2-1) can be approximated by

$$\mathbf{B}\boldsymbol{\phi}_\nu = \frac{1}{\nu}\boldsymbol{\phi}_\nu \tag{2.3}$$

where B is an $N \times N$ matrix defined by

$$\mathbf{B}_{i,j} \equiv \mu_i^{-1}\left(\delta_{i,j} - \frac{c}{2} f_{i,j} w_j\right), \qquad i, j = 1, 2, \ldots, N \tag{2.4}$$

and ν and $\boldsymbol{\phi}_\nu$ are, respectively, the eigenvalue and eigenvector. In Eq. (2.4) $\delta_{i,j}$ is the Kronecker delta symbol, μ_i and w_i the ith Gaussian quadrature point and corresponding Christoffel number respectively, and $f_{i,j}$ is given by

$$f_{i,j} \equiv f(\mu_i, \mu_j). \tag{2.5}$$

The discrete formulation of the eigenvalue problem of Eqs. (2.3) to (2.5) is essentially the discrete ordinate formulation of the problem studied by Chandrasekhar [8] without the expansion of the scattering function in Legendre polynomials. Based on Eq. (2.3), Odom [9] computed successfully the discrete eigenvalues ($\nu \notin (-1, 1)$) for several cases of anisotropic scattering. As the scattering function becomes increasingly peaked in the forward direction, the off-diagonal terms in **B** becomes increasingly smaller, and the retention of the diagonal and only a few neighboring off-diagonals in **B** is found to also yield good results.

Considerable computational effort can be avoided by converting the eigenvalue problem of Eq. (2.3) to one involving a matrix of a smaller rank. Towards this end, define a matrix **A** by

$$\mathbf{A}_{i,j} = \frac{1}{(2)^{1/2}} (\delta_{i,N+1-j} - \alpha_i \delta_{i,j})(\alpha_j \mu_j w_j)^{1/2}, \qquad i, j = 1, 2, \ldots, N \tag{2.6}$$

with

$$\begin{aligned} \alpha_i &= -1, \qquad \text{if } 1 \leqslant i \leqslant N/2 \\ &= \ \ 1, \qquad \text{if } N/2 < i \leqslant N. \end{aligned} \tag{2.7}$$

It is noted that the number of quadrature points N is assumed to be even and the μ_i's ($\mu_1 < \mu_2 < \cdots < \mu_N$) and the w_i's satisfy the conditions:

$$\alpha_i \mu_i = \alpha_{N+1-i} \mu_{N+1-i} > 0, \qquad w_i = w_{N+1-i} > 0, \qquad i = 1, 2, \ldots, N/2. \tag{2.8}$$

Further, since the azimuthally averaged scattering function has the property $f(\mu_i, \mu_j) = f(\mu_j, \mu_i) = f(-\mu_i, -\mu_j)$, it follows that

$$f_{i,j} = f_{j,i} = f_{N+1-i,N+1-j}, \qquad i, j = 1, 2, \ldots, N. \tag{2.9}$$

The inverse of **A** is given by

$$\mathbf{A}^{-1}_{i,j} = \frac{1}{(2)^{1/2}} \frac{1}{(\alpha_i \mu_i w_i)^{1/2}} (\delta_{i,N+1-j} - \alpha_i \delta_{i,j}), \tag{2.10}$$

and using this result and Eqs. (2.6) to (2.9) it is found that

$$(\mathbf{ABA}^{-1})_{i,j} = \tfrac{1}{2}[(\alpha_j - \alpha_i)\, \mathbf{P}_{i,j} + (\alpha_i \alpha_j - 1)\, \mathbf{P}_{i,N+1-j}] \tag{2.11}$$

with

$$\mathbf{P}_{i,j} \equiv \frac{1}{(\alpha_i \alpha_j \mu_i \mu_j)^{1/2}} \left(\delta_{i,j} - \frac{c}{2} f_{i,j} (w_i w_j)^{1/2}\right) \tag{2.12}$$

which has properties similar to those of $f_{i,j}$ as given by Eq. (2.9). Because the

matrices **B** and $\mathbf{ABA}^{-1}$ are related by a similarity transformation, they have identical eigenvalue spectra [10]. Furthermore, with the help of Eq. (2.7), it is seen that

$$[\mathbf{ABA}^{-1}]_{i,j} = 0 \tag{2.13}$$

if (1) $i \leqslant N/2$ and $j \leqslant N/2$, or (2) $i > N/2$ and $j > N/2$, and consequently

$$\mathbf{M}(\mathbf{ABA}^{-1})\,\mathbf{M}^{-1} = -\mathbf{ABA}^{-1} \tag{2.14}$$

with the matrix **M** and its inverse $\mathbf{M}^{-1}$ defined by

$$\mathbf{M}_{i,j} = \mathbf{M}^{-1}_{i,j} = \alpha_i \delta_{i,j}\,. \tag{2.15}$$

In other words, the matrix $\mathbf{ABA}^{-1}$ and its negative are related by a similarity transformation. Thus we conclude that, if λ ($\equiv 1/\nu$) is an eigenvalue of $\mathbf{ABA}^{-1}$, then so is $-\lambda$. Because $\mathbf{ABA}^{-1}$ is a real matrix, it follows that λ^* (the complex conjugate of λ) and $-\lambda^*$ must also be eigenvalues of $\mathbf{ABA}^{-1}$. All these conclusions, of course, apply also to the matrix **B**. In Appendix A it is shown that if $c(1 - \epsilon/2) < 1$ (where ϵ is the error obtained by evaluating $\int_{-1}^{1} d\mu'\, f(\mu, \mu')$ by numerical quadrature) then all the eigenvalues of **B** are necessarily real. However, it is found that for $c > 1$ some of the eigenvalues become imaginary or even complex.

If $\mathbf{ABA}^{-1}$ is written as

$$\mathbf{ABA}^{-1} = \begin{pmatrix} \mathbf{0} & \mathbf{E} \\ \mathbf{F} & \mathbf{0} \end{pmatrix} \tag{2.16}$$

with **E** and **F** two $N/2 \times N/2$ matrices, then it follows that

$$\mathbf{AB^2A}^{-1} = \begin{pmatrix} \mathbf{EF} & \mathbf{0} \\ \mathbf{0} & \mathbf{FE} \end{pmatrix}. \tag{2.17}$$

The implication of Eq. (2.17) is that, if λ is an eigenvalue of **B** then λ^2 must be an eigenvalue of one of the matrices **EF** or **FE**. If it is further assumed that the matrix **B** is nonsingular then it is easy to see that the matrices **EF** and **FE** are related by a similarity transformation and thus λ^2 must be an eigenvalue of both matrices **EF** and **FE**. As a matter of fact, it follows from Eq. (2.16) that both **E** and **F** must be nonsingular if **B** is nonsingular and thus

$$\mathbf{EF} = \mathbf{E}(\mathbf{FE})\,\mathbf{E}^{-1}. \tag{2.18}$$

In summary, it has been shown that if λ is an eigenvalue of **B** then λ^2 must be an eigenvalue of both matrices **EF** and **FE**. This fact coupled with the fact that the

eigenvalues of the matrix **B** appear in the combinations $\pm\lambda$, $\pm\lambda^*$ shows that, as far as the computation of eigenvalues is concerned, the $N/2 \times N/2$ matrix **EF** (or **FE**) is as useful as the larger $N \times N$ matrix **B**.

3. Numerical Considerations

Computer codes have been written to evaluate the discrete eigenvalues from the matrices **B** and **EF** using efficient matrix eigenvalue subroutines [11, 12]. As is to be expected the computations using the $N/2 \times N/2$ **EF** matrix is considerably faster than using the $N \times N$ **B** matrix (at least by a factor of three and even greater for large N), although identical results are obtained with both methods for the same order N of numerical quadrature. For a given quadrature N, the eigenvalues λ^2 of **EF** will not only contain some discrete eigenvalue but also some eigenvalues in the continuum ($\nu\epsilon(-1, 1)$); and as N increases eventually all discrete eigenvalues will be obtained and the continuum will begin to fill.

The matrix eigenvalue technique is very accurate for the calculation of those real discrete eigenvalues $|\nu| > 1.05$ and the complex discrete eigenvalues (for $c > 1$). In many cases very low quadrature orders are sufficient to obtain an accurate value of the asymptotic diffusion length (the largest ν). However for the calculation of the discrete eigenvalues close to unity, i.e., $|\nu| < 1.05$, the present technique requires that a high order numerical quadrature (and hence a large matrix size) be used. This effect is illustrated in Table I where the discrete eigenvalue

TABLE I

Discrete Eigenvalues for Isotropic Scattering
Matrix Method

c	$N = 8$	$N = 64$	Exact value
0.1	0.96607116	0.999444416428	1.000000004122
0.2	0.97440188	0.999893864352	1.000090886544
0.3	0.98720242	1.002591431962	1.002592888793
0.4	1.00773253	1.014585815901	1.014585815927
0.5	1.04223056	1.044382033761	1.044382033761
0.6	1.10169000	1.102132021151	1.102132021151
0.7	1.20675158	1.206804253985	1.206804253985
0.8	1.40763161	1.407634309063	1.407634309063
0.9	1.90320484	1.903204856045	1.903204856045
1.1	i 1.75665198	i 1.756651966318	i 1.756651966318
1.3	i 0.94600580	i 0.946000224918	i 0.946000224918

for isotropic scattering ($f \equiv 1$) as calculated by the matrix method is compared to the exact value (as computed from the explicit form of the dispersion function [5]) for various values of c.

To illustrate the application to highly anisotropic scattering situations the following fictitious scattering function is used [1, 13]

$$f(\Omega \cdot \Omega') \equiv \frac{M+1}{2^M}(1 + \Omega \cdot \Omega')^M, \qquad M = 0, 1, 2.... \tag{3.1}$$

This function becomes highly peaked in the forward direction as the index M increases, and has the useful property of being expandable into a $M + 1$ Legendre polynomial sum, i.e.

$$f(\Omega \cdot \Omega') = \sum_{m=0}^{M} b_m P_m(\Omega \cdot \Omega'), \tag{3.2}$$

where the expansion coefficients are given by

$$b_m = (2m + 1)\frac{M!(M+1)!}{(M-m)!\,(M+m+1)!}. \tag{3.3}$$

The azimuthally averaged scattering function, $f(\mu, \mu')$, is readily obtained from Eq. (3.2) by use of the addition theorem for Legendre polynomials.

The eight discrete eigenvalues for the case of $M = 200$ and $c = 0.95$ as computed by the matrix technique with various orders of numerical quadrature, N are

TABLE II

Discrete eigenvalues for $M = 200$ and $c = 0.95$ as calculated with the matrix technique and a Legendre expanded integral form of the dispersion relation [14].

	Legendre expansion[a]	Matrix technique $N = 16$	$N = 20$	$N = 24$	$N = 32$	$N = 64$
ν_1	1.02602204	—	—	—	1.024535	1.02602204
ν_2	1.12581670	1.01	1.15	1.135	1.125851	1.12581670
ν_3	1.32006749	1.58	1.38	1.132	1.320074	1.32006748
ν_4	1.66953495	2.05	1.71	1.672	1.669537	1.66953515
ν_5	2.31402373	2.72	2.35	2.316	2.314020	2.31401898
ν_6	3.59579677	4.15	3.64	3.598	3.595887	3.59588645
ν_7	6.44175667	7.47	6.50	6.443	6.440667	6.44066643
ν_8	13.5342422	16.16	13.67	13.544	13.540653	13.54065275

[a] Only first 99 Legendre coefficients were used for ν_1 to ν_7, and first 50 coefficients for the ν_8 calculation.

compared in Table II with those values computed with a conventional Legendre expanded integral form of the dispersion relation [1, 14]. For this example there are eight discrete eigenvalue pairs, and the values shown for $N = 64$ are estimated to be correct to eight significant figures. Notice that for small values of N the smaller discrete eigenvalues have the most error (in fact the smallest may be missed entirely). It has been found that generally the quadrature order used should be at least four times the number of discrete eigenvalue pairs for highly anisotropic situations ($N > 50$) to give the eigenvalues to within one percent accuracy. Generally the order, N, is increased until the eigenvalues remain unchanged with increasing order. For the $M = 200$ example, the Legendre expanded form of the dispersion relation yielded excellent values for the small eigenvalues, but very poor values for the large eigenvalues. This inaccuracy of the Legendre expansion technique is to be expected since, in the example given, a one hundred term expansion (50 for the largest eigenvalue) was used. The use of such large expansions requires the computation of sums of polynomials up to order 100 (or 50 for the largest eigenvalue) with arguments equal to the discrete eigenvalue to be accurately evaluated—a feat beyond the capability of current computers using standard programming techniques. Such numerical errors for the larger eigenvalues can, of course, be avoided by using a lower order approximation since there is generally rapid convergence of the larger eigenvalues with the order of the Legendre approximation [3, 15]. The direct technique however, avoids such numerical difficulties by not using Legendre expansions.

To verify the accuracy of the present technique, it is necessary to obtain an independent estimate of the diffusion length. Although for highly anisotropic situations and large diffusion lengths (c close to unity) the standard dispersion function approach is inadequate, a rapidly converging series expansion for the diffusion length can be used. Kuščer [16] reported the following expansion of the largest eigenvalue which has been found to be rapidly convergent as $c \to 1$:

$$\nu_0^{-2} \simeq h_0 h_1[1 - 4h_0/h_2 + h_0^2(16/h_2^2 - 36h_1/h_2^2 h_3 + O(h_0^3)] \tag{3.4}$$

where $h_m \equiv (2M + 1) - cb_m$. In Table III it is seen there is excellent agreement between values of the diffusion length as calculated by Eq. (3.4) (ignoring the $O(h_0^3)$ and higher order terms) and by the matrix technique for $M = 200$ as c approaches unity.

The matrix technique has been found to be significantly faster than the use of a fully Legendre expanded dispersion function [14] (typically a factor of ten) and, for large eigenvalues, capable of better accuracy. No difficulties are encountered as c becomes close to unity, and in fact, no special computational modifications are required if c becomes greater than unity and some of the discrete eigenvalues becomes imaginary or complex.

TABLE III

Diffusion length for $M = 200$ as calculated by a third order series expansion [16] and the matrix technique.

c	Series expansion	Matrix technique $N = 64$
.9	7.89	7.5873110
.99	45.16	45.223705
.999	177.2439	177.24474
.9999	578.13274	578.13272
.99999	1834.1805	1834.1805

APPENDIX

Under the conditions $c < 1$, all the eigenvalues of Eq. (2.3) are real if the value of N is chosen sufficiently large. To show this result first define

$$\epsilon_i \equiv \int_{-1}^{+1} f(\mu_i, \mu')\, d\mu' - \sum_{j=1}^{N} f_{i,j} w_j = 2 - \sum_{j=1}^{N} f_{i,j} w_j, \qquad i = 1,..., N. \quad \text{(A.1)}$$

If it is assumed that $f(\mu, \mu')$ is nonnegative and

$$c[1 - \epsilon_i/2] < 1, \qquad i = 1, 2,..., N. \quad \text{(A.2)}$$

then it is easy to see that

$$\sum_{j=1}^{N} \frac{|(c/2) f_{i,j}(w_i w_j)^{1/2}|}{(w_i)^{1/2}} (w_j)^{1/2} < 1, \qquad i = 1, 2,..., N. \quad \text{(A.3)}$$

To proceed further, the following theorem is used [17]:

THEOREM. *If* $\mathbf{A}$ *is an arbitrary* $N \times N$ *complex matrix, and* $x_1, x_2,..., x_N$ *are* N *positive numbers, let*

$$\tau \equiv \max_{1 \leqslant i \leqslant N} \left\{ \frac{\sum_{j=1}^{N} |\mathbf{A}_{i,j}| X_j}{X_i} \right\},$$

then, $\rho(\mathbf{A}) \leqslant \tau$, *with* $\rho(\mathbf{A}) \equiv$ *spectral radius of* $\mathbf{A}$.

From this theorem, Eq. (A.3) implies that

$$\rho(\mathbf{I} - \mathbf{S}) < 1 \quad \text{(A.4)}$$

where **I** is the $N \times N$ identity matrix and **S** a $N \times N$ matrix defined by

$$\mathbf{S}_{i,j} = \delta_{i,j} - \frac{c}{2} f_{i,j} (w_i w_j)^{1/2}. \tag{A.5}$$

If σ is any eigenvalue of **S**, then Eq. (A.4) implies that

$$| 1 - \sigma | < 1. \tag{A.6}$$

Because the matrix **S** is real and symmetric, σ must be real. This result coupled with Eq. (A.6) implies that σ is positive, and it follows that the matrix **S** is real, symmetric and positive–definite. A matrix with these properties has a uniquely defined square root which also possesses these properties [18]. In other words, there exists a real, symmetric and positive–definite matrix $\mathbf{S}^{1/2}$ such that

$$\mathbf{S}^{1/2}\mathbf{S}^{1/2} = \mathbf{S} \tag{A.7}$$

From a straightforward calculation it is found that **B** is related to a real symmetric by a similarity transformation, namely

$$(\mathbf{S}^{1/2}\mathbf{W})\, \mathbf{B} (\mathbf{S}^{1/2}\mathbf{W})^{-1} = \mathbf{S}^{1/2}\boldsymbol{\mu}^{-1}\mathbf{S}^{1/2} \tag{A.8}$$

with the diagonal matrices **W** and $\boldsymbol{\mu}$ defined by

$$\mathbf{W}_{i,j} = \sqrt{w_i}\, \delta_{i,j}\,, \tag{A.9}$$

and

$$\mu_{i,j} = \mu_i\, \delta_{i,j} \tag{A.10}$$

Because the eigenvalue spectrum of the real symmetric matrix $S^{1/2}\boldsymbol{\mu}^{-1}\mathbf{S}^{1/2}$ is real, then so is that of the matrix **B**.

Finally it is noted that

$$\lim_{N\to\infty} \epsilon_i = 0, \qquad i = 1, 2, \ldots, N \tag{A.11}$$

and thus if $c < 1$, Eq. (A.2) can always be realized by choosing N sufficiently large.

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