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ON COMPUTING THE CHANDRASEKHAR POLYNOMIALS IN HIGH ORDER AND HIGH DEGREE

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Abstract—The polynomials $g_l^m(\xi)$ introduced by Chandrasekhar in regard to a discrete-ordinates solution of the radiative transfer equation are discussed, and methods for evaluating these polynomials accurately in high order and high degree on the real line are reported.

1. INTRODUCTION

In his classic work on a radiative transfer, Chandrasekhar[1] introduced a new class of polynomials in regard to his discrete-ordinates solution of the equation of transfer. These polynomials, to which we refer as the Chandrasekhar polynomials or the g polynomials, have also been found to play a fundamental role in other analytical and computational methods in radiative transfer. In particular some versions of the spherical harmonics method,[2,3] the method of elementary solutions,[4,5] and the F_N method[6,7] all require the g polynomials in one way or another. Analytical properties of the Chandrasekhar polynomials have been discussed in detail by İnönü[8] for the azimuthally symmetric case ($m = 0$). In addition there has been some discussion[9–11] in regard to the difficulty in computing these polynomials accurately for the general case ($m \geqslant 0$).

We define the *normalized* Chandrasekhar polynomials $g_l^m(\xi)$ with the starting value

$$g_m^m(\xi) = (2m - 1)!![(2m)!]^{-1/2} \tag{1}$$

and the three-term recursion relation

$$(l^2 - m^2)^{1/2} g_{l-1}^m(\xi) - h_l \xi g_l^m(\xi) + [(l+1)^2 - m^2]^{1/2} g_{l+1}^m(\xi) = 0 \tag{2}$$

for $\geqslant m$. Here

$$h_l = 2l + 1 - \varpi\beta_l, \quad l = 0, 1, \ldots, L, \tag{3a}$$

and

$$h_l = 2l + 1, \quad l > L, \tag{3b}$$

where $\varpi \in (0, 1]$ is the albedo for single scattering and the β_l, for $l = 0, 1, 2, \ldots, L$, are the coefficients in an Lth-order Legendre expansion of the scattering law.[3]

In this work, we discuss methods for computing accurately the Chandrasekhar polynomials $g_l^m(\xi)$ for $\xi \in \mathscr{R}$. Clearly, $g_l^m(-\xi) = (-1)^{l-m} g_l^m(\xi)$, and so we restrict our attention to $\xi \geqslant 0$. We consider that the polynomials $g_l^m(\xi)$ are required for $m = 0, 1, \ldots, L$ and $l = m, m + 1, \ldots, L$.

2. COMPUTATIONAL METHODS

We consider initially that $\varpi \neq 1$ when $m = 0$; the modifications required to handle the special case $\varpi = 1$ and $m = 0$ will be reported at the end of this section. For $\xi \in [0, 1]$ we follow Gautschi[12] and use Eq. (2) in the forward direction to generate the required $g_l^m(\xi)$ without significant loss of accuracy (except near a zero of one of the polynomials). We note that for $\xi \to 1$ the g polynomials approach very large values in high order and high degree, and so we have used two arrays in computer calculations to store the required $g_l^m(\xi)$—one for the mantissa and another for the exponent—in order to avoid computer overflows.

In a previous paper,[13] we used Sturm sequences to compute the discrete spectrum basic to several analytical and computational methods in radiative transfer. This spectrum, which is composed of the so-called discrete eigenvalues, is defined on the half plane $\mathscr{R}\, z > 0$ as the zeros ($\nu_\alpha^0 > 1$, and $\nu_\alpha^m \geq 1$, for $m \geq 1$, $\alpha = 1, 2, \ldots, \aleph^m$) of the dispersion function

$$\Lambda^m(z) = 1 - z \int_{-1}^{1} \psi^m(\mu) \frac{d\mu}{z - \mu} \tag{4}$$

where the characteristic function is

$$\psi^m(\mu) = \frac{\varpi}{2}(1 - \mu^2)^{m/2} \sum_{l=m}^{L} \beta_l g_l^m(\mu) P_l^m(\mu) \tag{5}$$

and we use

$$P_l^m(\mu) = \left[\frac{(l-m)!}{(l+m)!}\right]^{1/2} (1 - \mu^2)^{m/2} \frac{d^m}{d\mu^m} P_l(\mu) \tag{6}$$

to denote the normalized associated Legendre functions.

Considering now that we wish to compute the Chandrasekhar polynomials $g_l^m(\xi)$ for $\xi = \nu_\alpha^m$, $\alpha = 1, 2, \ldots, \aleph^m$, we note that in the past we have used[7] backward recurrence for this case since the $g_l^m(\nu_\alpha^m)$ approach zero as $l \to \infty$. Defining the ratios

$$G_l^m(\nu_\alpha^m) = \frac{g_{l+1}^m(\nu_\alpha^m)}{g_l^m(\nu_\alpha^m)}, \tag{7}$$

we have,[7] in the spirit of Gautschi,[12] used for starting value $G_M^m(\xi) = 0$ for some $M > L$ and

$$G_{l-1}^m(\xi) = (l^2 - m^2)^{1/2}\{h_l \xi - [(l+1)^2 - m^2]^{1/2} G_l^m(\xi)\}^{-1} \tag{8}$$

for $l = M, M-1, \ldots, m+1$, to compute the desired ratios for the case $\xi = \nu_\alpha^m$, $\alpha = 1, 2, \ldots, \aleph^m$. We then used increasing values of M until the computed values of the ratios $G_l^m(\xi)$ for $l = m, m+1, \ldots, L-1$ ceased to change. Of course once the ratios are known, we can find the g polynomials, for the case $\xi = \nu_\alpha^m$, $\alpha = 1, 2, \ldots, \aleph^m$, from the starting value given by Eq. (1) and

$$g_{l+1}^m(\xi) = G_l^m(\xi) g_l^m(\xi) \tag{9}$$

for $l = m, m+1, \ldots, L-1$.

Although we have used this scheme of backward recursion to obtain accurate results for the g polynomials for numerous applications, we have recently found problems for which this approach can fail to yield the desired results accurately. In particular, while trying to solve the *cloud problem* of Ref. 7 for the case of a non-normally incident beam, which requires that all ($m = 0, 1, \ldots, L = 299$) Fourier component problems be solved, we found that the ratios $G_l^m(\xi)$ could become > 1 in absolute value as $l \to m$ and subsequently that round-off errors could start to accumulate until all significant figures were lost.

Having found that there are cases where the foregoing scheme of backward recursion can fail, we now summarize an improved algorithm for computing the Chandrasekhar polynomials on the discrete spectrum. First of all we compute the starting ratio

$$G_L^m(\nu_\alpha^m) = \frac{g_{L+1}^m(\nu_\alpha^m)}{g_L^m(\nu_\alpha^m)} \tag{10}$$

from the equivalent expression

$$G_L^m(\nu_\alpha^m) = \frac{Q_{L+1}^m(\nu_\alpha^m)}{Q_L^m(\nu_\alpha^m)} \tag{11}$$

as described in Ref. 13. Here the Q functions are defined[13] by

$$Q_l^m(\xi) = \frac{1}{2} \int_{-1}^{1} (1 - \mu^2)^{m/2} P_l^m(\mu) \frac{d\mu}{\xi - \mu}. \tag{12}$$

Next we use Eq. (8) in the backward direction only as long as the $|G_l^m(\nu_\alpha^m)| < 1$. To be specific, suppose this is true for $l = L-1, L-2, \ldots, L^*$, but false for L^*-1. Then we stop the backward recursion and switch to forward recursion. We use Eq. (2) for $l = m, m+1, \ldots,$ as long as $|G_l^m(\nu_\alpha^m)| \geqslant 1$. Suppose we can use Eq. (2) for $l = m, m+1, \ldots, l^*-1$, so that we have computed $g_m^m(\nu_\alpha^m)$, $g_{m+1}^m(\nu_\alpha^m), \ldots, g_{l^*}^m(\nu_\alpha^m)$, and then we find $|G_{l^*}^m(\nu_\alpha^m)| < 1$. In this case we stop the forward recursion and, if $l^* \leqslant L^*-1$, we compute the polynomials $g_{l^*+1}^m(\nu_\alpha^m)$, $g_{l^*+2}^m(\nu_\alpha^m), \ldots, g_{L^*}^m(\nu_\alpha^m)$ by first solving a linear system obtained from Eq. (2) for $l = l^*+1, l^*+2, \ldots, L^*$ and expressed as

$$\mathbf{A}^m(\nu_\alpha^m)\mathbf{f}^m(\nu_\alpha^m) = \mathbf{b}^m(\nu_\alpha^m), \tag{13}$$

where $\mathbf{A}^m(\nu_\alpha^m)$ is a symmetric tridiagonal matrix, or order (L^*-l^*), that has the elements

$$-h_{l^*+1}\nu_\alpha^m,\ -h_{l^*+2}\nu_\alpha^m, \ldots,\ -h_{L^*-1}\nu_\alpha^m,\ -h_{L^*}\nu_\alpha^m + [(L^*+1)^2 - m^2]^{1/2} G_{L^*}^m(\nu_\alpha^m)$$

on the diagonal and the elements

$$[(l^*+2)^2 - m^2]^{1/2}, [(l^*+3)^2 - m^2]^{1/2}, \ldots, [(L^*)^2 - m^2]^{1/2}$$

on the sub- and super-diagonals, the vector $\mathbf{f}^m(\nu_\alpha^m)$ has components

$$g_{l^*+1}^m(\nu_\alpha^m)/g_{l^*}^m(\nu_\alpha^m),\ g_{l^*+2}^m(\nu_\alpha^m)/g_{l^*}^m(\nu_\alpha^m), \ldots, g_{L^*}^m(\nu_\alpha^m)/g_{l^*}^m(\nu_\alpha^m)$$

and $\mathbf{b}^m(\nu_\alpha^m)$ has components

$$-[(l^*+1)^2 - m^2]^{1/2}, 0, \ldots, 0,$$

and then multiplying the resulting $\mathbf{f}^m(\nu_\alpha^m)$ by $g_{l^*}^m(\nu_\alpha^m)$. Finally we can readily use the ratios computed by backward recursion of Eq. (8) and $g_{L^*}^m(\nu_\alpha^m)$ in Eq. (9) with $l = L^*, L^*+1, \ldots, L-1$ in order to compute the remaining $g_{L^*+1}^m(\nu_\alpha^m), g_{L^*+2}^m(\nu_\alpha^m), \ldots, g_L^m(\nu_\alpha^m)$.

We note that in the event the Chandrasekhar polynomials are required for $\xi > 1$, $\xi \neq \nu_\alpha^m$, $\alpha = 1, 2, \ldots, \aleph^m$, as, for example, when solving multigroup radiation transport problems,[14,15] we use the starting value given by Eq. (1) and the Darboux formula

$$g_{l+1}^m(\xi) = G_l^m(\eta) g_l^m(\xi) + \frac{\xi - \eta}{[(l+1)^2 - m^2]^{1/2} g_l^m(\eta)} \sum_{k=m}^{l} h_k g_k^m(\eta) g_k^m(\xi) \tag{14}$$

for $l = m, m+1, \ldots, L-1$ to generate the required $g_l^m(\xi)$, $l = m, m+1, \ldots, L$. Here we choose η to be the discrete eigenvalue closest to ξ (we take $\eta = 1$ if there are no discrete eigenvalues) and we use, as we did when computing the g polynomials for $\xi \in [0, 1]$, two arrays in computer calculations to store the required $g_l^m(\xi)$, in order to avoid underflows and overflows. In contrast to schemes based on forward recursion of Eq. (2), our present method based on Eq. (14) is particularly effective when ξ is close to a discrete eigenvalue.

To conclude this section, we report here some modifications required in order to compute the g polynomials for the special case $\varpi = 1$ and $m = 0$. We note that in this case we have $g_0^0(\xi) = 1$, $g_1^0(\xi) = 0$ and $g_2^0(\xi) = -1/2$, and so when computing the g polynomials for the bounded discrete eigenvalues we should use backward recursion of Eq. (8) only for $l = L, L-1, \ldots, 3$ (and, of course, only as long as the ratio $|G_l^m(\nu_\alpha^m)| < 1$). In case we need to switch to forward recursion, and, if necessary, to solve a linear system analogous to Eq. (13), to complete the calculation, we note that Eq. (2) should be used only for $l \geqslant 2$. In addition, we note that when computing the g polynomials for $\varpi = 1$, $m = 0$ and $\xi > 1$, $\xi \neq \nu_\alpha^m$, $\alpha = 1, 2, \ldots, \aleph^m$, we should use Eq. (14) only for $l = 2, 3, \ldots, L-1$.

3. NUMERICAL IMPLEMENTATION AND DISCUSSION

We have programmed and implemented our methods for computing the Chandrasekhar polynomials on a CDC CYBER 170/750 computer and on an IBM-PC. We used two scattering laws in order to test the developed methods: the $L = 299$ *cloud* phase function for which Legendre coefficients are tabulated in Refs. 3 and 7 and the binomial scattering law[16]

$$p(\cos\Theta) = \frac{L+1}{2^L}(1 + \cos\Theta)^L. \tag{15}$$

This scattering law can be represented exactly with $(L+1)$ Legendre coefficients that can be computed with $\beta_0 = 1$ and

$$\beta_l = \left(\frac{2l+1}{2l-1}\right)\left(\frac{L+1-l}{L+1+l}\right)\beta_{l-1} \tag{16}$$

for $l = 1, 2, \ldots, L$. We note that we should have pointed out in Ref. 13 that the useful recursion formula given in Eq. (16) was previously reported by McCormick and Sanchez.[17] In our tests with this scattering law we also used $L = 299$.

We computed the Chandrasekhar polynomials $g_l^m(\xi)$, $m = 0, 1, \ldots, L$ and $l = m, m+1, \ldots, L$, for both scattering laws and single scattering albedos that varied from 0.1 to 1.0 in steps of 0.1 on a grid defined by $\xi = 0.0(0.1)1.0$, $\xi = \nu_\alpha^m(1 \pm 10^{-s})$, $\alpha = 1, 2, \ldots, \aleph^m$ and $s = 5$, 10, 15 and ∞, and $\xi = 1 + 2^t/10$, $t = 0, 1, \ldots, 8$. By comparing the results of our tests done in single and double precision on the CYBER machine, we concluded that the procedure described in Sec. 2 is capable of providing the Chandrasekhar polynomials with good accuracy (loss of $\leqslant 4$ significant figures except very close to the zeros of the polynomials) for a class of scattering laws characterized by strong anisotropy.

A few comments on specific points of our procedure to compute the g polynomials for the discrete spectrum are in order. We have used the LINPACK[18] subroutines SGBCO and SGBSL (and their double precision versions) to solve the linear system defined by Eq. (13). By monitoring the condition estimates returned by SGBCO, we found that the linear systems appeared to be always relatively well conditioned, so that we found solutions that had, in most cases, only 2 or 3 fewer significant figures of accuracy than the matrix elements. In the event we do not wish to monitor the condition number of our linear system, one of the LINPACK subroutines SGTSL (single precision) or DGTSL (double precision) can be used to solve the linear system more quickly.

In addition, for each m component for which discrete eigenvalues were present, we found that the size of the linear system varied monotonically from 0 (for the largest discrete eigenvalue) to a maximum value (for the smallest discrete eigenvalue) that depended on how close to 1 the smallest discrete eigenvalue was—there were cases where we had to solve linear system of size near 200.

We also compared the results of our method for computing the g polynomials for the discrete spectrum with results from the inverse iteration procedure of Wilkinson,[19] as implemented in the EISPACK package[20] (subroutine TINVIT). Despite the fact that the inverse iteration procedure cannot yield accurately eigenvector components that have the ratio of their magnitudes to the magnitude of the largest component smaller than the machine precision, the inverse iteration results looked very good when we used any of the usual vector norms[21] to measure their deviations from the results of our method. However, when we tried to use the inverse iteration results in Eq. (14) to generate the polynomials $g_l^m(\xi)$ off the discrete spectrum, we observed disastrous results as $l \to L$ and so we concluded that inverse iteration cannot be used when one is interested in computing the g polynomials for $\xi > 1$, $\xi \neq \nu_\alpha^m$, $\alpha = 1, 2, \ldots, \aleph^m$. Even if this calculation is not required, our procedure has the advantages of not being iterative and of involving the solution of a linear system of reduced size when compared with the inverse iteration procedure.

Finally, we should like to point out that our work was developed having in mind the Chandrasekhar polynomials as required by methods that make use of the "exact" discrete spectrum, i.e., the zeros of Eq. (4), for solving the radiative transfer equation. Clearly, our work can be easily adapted to generate the Chandrasekhar polynomials for spherical harmonics methods[2,3] of order $N-1$ and discrete ordinates methods[1,22] of order N that use the zeros of $g_N^m(\xi)$ with magnitudes > 1 to approximate the "exact" discrete spectrum. To this end, all that we need to do is to work with the "approximate" discrete spectrum instead of the "exact" discrete spectrum and to take zero as the starting ratio for backward recursion of Eq. (8).

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