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ON COMPUTING A CLASS OF INTEGRALS BASIC TO THE F_N METHOD IN RADIATIVE TRANSFER

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Abstract—Methods for computing a class of integrals basic to the F_N method in radiative transfer are discussed. New recursion relations are derived and used to develop an improved computational scheme for calculating these integrals accurately in high degree.

1. INTRODUCTION

Computationally speaking, we note that radiative transfer through a thick cloud is one of the more difficult problems in the field of particle transport theory. Among the methods that have been applied to solve this problem,[1] the F_N method[2–4] has been perhaps the most successful, as demonstrated by the quality of the results[4] generated with the method for some model problems posed by the International Association of Meteorology and Atmospheric Physics.

Although effective for the problems solved in Ref. 4, we have found that the F_N method still requires improvement in a few numerical aspects before it can be applied to more challenging problems (i.e., problems with even larger degrees of anisotropy). Recently, we have reported new effective methods for computing the discrete spectrum associated with the equation of transfer[5] and for computing the Chandrasekhar polynomials.[6] In this paper, we report some recent developments in our continuing work on computational methods that we hope will end up in extending the range of applicability of the F_N method to more demanding calculations.

The F_N method for solving radiative transfer problems without azimuthal symmetry has been discussed in detail in previous works.[2–4] One of the basic requirements of the method is that the integrals

$$T^m_{\alpha,l} = \int_0^1 \mu(1-\mu^2)^{m/2} P_\alpha(2\mu - 1) P^m_l(\mu)\,d\mu \tag{1}$$

be computed for $m = 0, 1, \ldots, L$ and $l = m, m+1, \ldots, L$, where L is the order of the phase function, and $\alpha = 0, 1, \ldots, N$, where N is the order of the F_N approximation. Here, as in Refs. 2–4, we define the associated Legendre functions as

$$P^m_l(\mu) = (1-\mu^2)^{m/2} \frac{d^m}{d\mu^m} P_l(\mu). \tag{2}$$

Computational methods for evaluating the required $T^m_{\alpha,l}$ integrals have been proposed in Refs. 3 and 4. In Ref. 3, a recursive scheme based on a five-term recursion relation was proposed. Later,[4] the scheme of Ref. 3 was found to be unstable as $m \to \infty$ so that, as a result of the propagation of roundoff errors, the computed values of the $T^m_{\alpha,l}$ integrals were not sufficiently accurate for m bigger than about 70. A recursive scheme based on the use of the five-term recursion relation of Ref. 3 for $m = 0$ and a three-term recursion relation relating $T^{m+1}_{\alpha,l}$ to $T^m_{\alpha,l-1}$ and $T^m_{\alpha,l+1}$ was then proposed to overcome this problem.[4] Unfortunately, we have found that, although slightly superior to the scheme of Ref. 3, the method of Ref. 4 is also unstable as $m \to \infty$.

Here we develop a new method for evaluating the $T^m_{\alpha,l}$ integrals that does not suffer from the limitations of the previous schemes[3,4] for problems that involve large values of m. Thus, our new scheme can be employed with confidence when solving problems with highly anisotropic scattering and azimuthal dependence. We note, for example, that the Cloud C_1 problem of Ref. 1 would involve such large values of m if we were to consider a non-normally incident beam of radiation.

The outline of this paper is as follows. In Sec. 2, we report some newly developed recursion relations for the $T^m_{\alpha,l}$ integrals. In Sec. 3, we show how these recursion relations can be combined to obtain an especially accurate computational scheme for calculating the $T^m_{\alpha,l}$ integrals and, finally, in Sec. 4 we discuss aspects of the numerical implementation of our computational scheme and present our concluding remarks.

2. RECURSION RELATIONS

To start this section, we point out that the task of computing the required $T^m_{\alpha,l}$ integrals can be greatly reduced if we observe that, since $\mu(1-\mu^2)^{m/2}P^m_l(\mu)$ is a polynomial of degree $(l+m+1)$, it is clear from the definition of $T^m_{\alpha,l}$ and the orthogonality property of the Legendre polynomials that $T^m_{\alpha,l}=0$ for $\alpha > l+m+1$.

In addition, a series representation for $T^m_{\alpha,l}$ can be easily found if we substitute

$$P_\alpha(2\mu-1)=\sum_{k=0}^{\alpha}(-1)^{\alpha+k}\frac{(\alpha+k)!}{(\alpha-k)!(k!)^2}\mu^k \tag{3}$$

into Eq. (1). The resulting integrals[2] are tabulated (see formula 7.132.5 of Gradshteyn and Ryzhik[7]) and so we find

$$T^m_{\alpha,l}=2^{-m-1}\left[\frac{(l+m)!}{(l-m)!}\right]\sum_{k=0}^{\alpha}(-1)^{\alpha+k}\frac{(\alpha+k)!}{(\alpha-k)!(k!)^2}\frac{\Gamma\left(\frac{k}{2}+1\right)\Gamma\left(\frac{k}{2}+\frac{3}{2}\right)}{\Gamma\left(\frac{k+l+m}{2}+2\right)\Gamma\left(\frac{k-l+m}{2}+\frac{3}{2}\right)}. \tag{4}$$

Although the series expressed by Eq. (4) could be used, in principle, to compute the $T^m_{\alpha,l}$ integrals, this idea should be discarded when one considers both the number of operations required and the problem of summing up accurately long alternating series composed of nearly cancelling terms. Nevertheless, Eq. (4) can be used to show that the $T^m_{\alpha,l}$ integrals, for $\alpha \geqslant 1$, satisfy the four-term recursion relation

$$\begin{aligned}(2+\alpha+l+m)T^m_{\alpha,l}=(2-\alpha+l+m)T^m_{\alpha-1,l}+\left[\frac{(l+m-1)(l+m)}{(l-m-1)(l-m)}\right]\\ \times[(3+\alpha-l+m)T^m_{\alpha,l-2}-(3-\alpha-l+m)T^m_{\alpha-1,l-2}]\end{aligned} \tag{5}$$

which is certainly more convenient than Eq. (4) from a computational point-of-view. Clearly, the first two columns ($l=m$ and $l=m+1$) and the first row ($\alpha=0$) of the $\mathbf{T}^m$ matrix are needed to start using Eq. (5). We can find a general recursion formula relating any column of the $\mathbf{T}^m$ matrix to a corresponding column of the $\mathbf{T}^{m-1}$ matrix if we use[4]

$$(2l+1)T^{m+1}_{\alpha,l}=(l+m)(l+m+1)T^m_{\alpha,l-1}-(l-m)(l-m+1)T^m_{\alpha,l+1} \tag{6}$$

twice to eliminate $T^m_{\alpha,l}$ and $T^m_{\alpha-1,l}$ from Eq. (5). After a rearrangement of indices, we find

$$(2+\alpha+l+m)T^m_{\alpha,l}=(2-\alpha+l+m)T^m_{\alpha-1,l}+(l+m-1)(l+m)[T^{m-1}_{\alpha,l-1}-T^{m-1}_{\alpha-1,l-1}] \tag{7}$$

which, for $\alpha \geqslant 1$, can be used for all $l \geqslant m$ when $m \geqslant 1$, but only for $l=0$ and 1 when $m=0$.

Another useful recursion relation for the $T^m_{\alpha,l}$ integrals can be obtained if we subtract Eq. (1) with $l \Leftarrow l-1$ from Eq. (1) with $l \Leftarrow l+1$ and use the recursion relations

$$P^m_{l+1}(\mu)-P^m_{l-1}(\mu)=(2l+1)(1-\mu^2)^{1/2}P^{m-1}_l(\mu) \tag{8a}$$

and

$$(\alpha+1)P_{\alpha+1}(2\mu-1)+\alpha P_{\alpha-1}(2\mu-1)=(2\alpha+1)(2\mu-1)P_\alpha(2\mu-1) \tag{8b}$$

along with

$$1-\mu^2=\tfrac{1}{4}[3-2(2\mu-1)-(2\mu-1)^2] \tag{9}$$

and Eqs. (5), (6) and (7). We find, after carrying out rather extensive algebraic manipulations, that we can, for $m \geqslant 0$, $l \geqslant m$, and $\alpha \geqslant 1$, write

$$\Gamma^m_{\alpha,l}T^m_{\alpha+2,l} - \Lambda^m_{\alpha,l}T^m_{\alpha+1,l} - \Upsilon^m_{\alpha,l}T^m_{\alpha,l} + \Upsilon^m_{-\alpha,l}T^m_{\alpha-1,l} + \Lambda^m_{-\alpha,l}T^m_{\alpha-2,l} - \Gamma^m_{-\alpha,l}T^m_{\alpha-3,l}$$
$$= 4(1-\delta_{l,m})(1-\delta_{l,m+1})\left[\frac{(l+m-1)(l+m)}{2l-1}\right][T^m_{\alpha,l-2} - T^m_{\alpha-1,l-2}], \quad (10)$$

where

$$\Gamma^m_{\alpha,l} = \left[\frac{(\alpha+1)(\alpha+2)}{(2\alpha+1)(2\alpha+3)}\right](4+\alpha+l+m), \quad (11a)$$

$$\Lambda^m_{\alpha,l} = \left(\frac{\alpha+1}{2\alpha+1}\right)\left[\left(\frac{\alpha}{2\alpha-1}\right)(4-\alpha+l+m) - 2(4+\alpha+l+m)\right] \quad (11b)$$

and

$$\Upsilon^m_{\alpha,l} = \frac{1}{2}\left[3 - \frac{1}{(2\alpha-1)(2\alpha+3)}\right](4+\alpha+l+m) + \left(\frac{1}{2\alpha-1}\right)(4-\alpha+l+m) - 2(2m-1)\left(\frac{l+m}{2l-1}\right). \quad (11c)$$

3. COMPUTATIONAL SCHEME

In the previous section, we have presented some new recursion formulas developed for the $T^m_{\alpha,l}$ integrals. The next task we undertook in our work was to verify whether or not any of the newly developed recursion formulas, i.e. Eqs. (5), (7) and (10), could be the basis of a stable scheme for computing the required $T^m_{\alpha,l}$. After extensive testing of all these formulas, we concluded that none is stable as $m \to \infty$.

In our search of a stable scheme for computing the required $T^m_{\alpha,l}$, we then followed the approach of looking for ways of reducing the dimensionality of the calculation. We note that the problem of computing the $T^m_{\alpha,l}$ integrals is originally defined in a tridimensional space (α-l-m) and that the recursive schemes of Refs. 3 and 4 work in bidimensional spaces (α-l and l-m respectively); however neither of these schemes is stable, as discussed in the Introduction. Here, two of the new formulas [Eqs. (5) and (10)] also work in the α-l space while the other [Eq. (7)] works in the full α-l-m space. However, by combining Eqs. (5) and (10), we were able to deduce a seven-term recursion relation for $T^m_{\alpha,l}$ that works in the α space, thereby allowing the entire calculation to be reduced to several one-dimensional calculations. To give an idea of the procedure we used to obtain the one-dimensional recursion formula just mentioned, we first rewrite Eq. (10) as

$$Y^m_{\alpha,l} = 4(1-\delta_{l,m})(1-\delta_{l,m+1})\left[\frac{(l+m-1)(l+m)}{2l-1}\right][T^m_{\alpha,l-2} - T^m_{\alpha-1,l-2}], \quad (12)$$

where $Y^m_{\alpha,l}$ denotes the left-hand side of Eq. (10). Using Eqs. (5) and (12) as they are and also with $\alpha \Leftarrow \alpha+1$, we do obtain, after some algebraic manipulations, the desired result, i.e.

$$\alpha(4+\alpha-l+m)Y^m_{\alpha+1,l} - (\alpha+1)(3-\alpha-l+m)Y^m_{\alpha,l} = 4\left[\frac{(l-m-1)(l-m)}{2l-1}\right]$$
$$\times [\alpha(3+\alpha+l+m)T^m_{\alpha+1,l} - (2\alpha+1)(l+m+2)T^m_{\alpha,l} + (\alpha+1)(2-\alpha+l+m)T^m_{\alpha-1,l}]. \quad (13)$$

We now describe our scheme for computing the $T^m_{\alpha,l}$ integrals. First we note that, since the right-hand side of Eq. (10) vanishes for $l=m$ and $l=m+1$, Eq. (10) constitutes a one-dimensional formula which is more convenient than Eq. (13) for computing the first two columns of the $\mathbf{T}^m$ matrix. Indeed, given the initial values $T^m_{2m+1,m}$ and $T^m_{2m+2,m+1}$ (computed as shown later in this section), we have found that Eq. (10) can be used in the backward direction for $\alpha = l+m+3$, $l+m+2, \ldots, 3$ and $l=m$ and $l=m+1$, to compute the first two columns of the $\mathbf{T}^m$ matrix accurately, for m up to 299.

In regard to the remaining columns ($m+2 \leqslant l \leqslant L$) of the $\mathbf{T}^m$ matrix, we first note that the right-hand side of Eq. (10) also vanishes for $\alpha = l+m+3$, $l+m+2$ or $l+m+1$. Therefore, to compute each of these columns, we used the initial value $T^m_{l+m+1,l}$ (computed as shown later in this section), Eq. (10) in the backward direction for the three mentioned values of α and then Eq. (13) in the backward direction for $\alpha = l + m,\ l + m - 1, \ldots, 3 + I_l^m$, where $I_l^m \geqslant 0$ depends on the column being computed, as explained next. Of course, it would be nice if we could always use Eq. (13) in the backward direction all the way down to $\alpha = 3$. However, it is usually necessary to terminate backward recursion of Eq. (13) prematurely ($I_l^m > 0$) because the absolute values of $T_{\alpha,l}^m$ tend to saturate when $\alpha \to 0$; if Eq. (13) continues to be used in the backward direction under these conditions, the accuracy of the calculation can be severely affected by the propagation of roundoff errors.

The value of I_l^m for which backward recursion of Eq. (13) should be stopped is, to some extent, arbitrary. It may depend, among other things, on the degree of accuracy desired for the $T_{\alpha,l}^m$ and also on the precision of the machine used to implement the calculation. To decide when to stop backward recursion of Eq. (13), we used the strategy of carrying out two calculations in parallel; in one of them we applied a perturbation, multiplying the starting value $T_{l+m+1,l}^m$ by $(1 + \epsilon)$, where the factor ϵ was taken as a small multiple of the machine precision for floating-point arithmetic. Since we have found that sometimes the perturbation applied on the starting value was damped as the calculation progressed, we have also multiplied by $(1 + \epsilon)$ any subsequent perturbed term that came out exactly equal to its unperturbed counterpart in the computer. The relative deviations between the $T_{\alpha,l}^m$ obtained from both calculations were continually monitored and backward recursion interrupted if a deviation bigger than δ (another prescribed factor $> \epsilon$) happened twice consecutively. For the columns of the $\mathbf{T}^m$ matrix where this happened before α reached 3, we defined $I_l^m = \alpha^* - 1$, with α^* denoting the current value of α in the program, and then switched to forward recursion of Eq. (13). As a general rule, we observed that the values of I_l^m tend to increase as $l \to L$; it was always possible, however, to compute the majority of the terms in a column by backward recursion of Eq. (13). In order to complete the calculation for the columns where $I_l^m > 0$, we computed the first four rows ($0 \leqslant \alpha \leqslant 3$) of the $\mathbf{T}^m$ matrix as discussed later in this section and then used Eq. (13) for $\alpha = 1, 2, \ldots, I_l^m - 4$. As before, we carried out the forward calculation twice in parallel (with one of the calculations being subject to a perturbation) and made a provision for warning message displays during program execution any time a deviation bigger than δ occurred twice consecutively between both calculations.

We now discuss our methods for computing the initial values required for backward and forward recursion of Eq. (13). For backward recursion, we require the last non-null elements of all the columns of the $\mathbf{T}^m$ matrix, i.e. $T_{l+m+1,l}^m$, $l = m, m + 1, \ldots, L$. If we let $l \Leftarrow l - 1$ and set $\alpha = l + m + 1$ in the recursion relation[3]

$$(l - m + 1)T_{\alpha,l+1}^m = \left(\frac{2l+1}{2}\right)\left[\left(\frac{\alpha}{2\alpha+1}\right)T_{\alpha-1,l}^m + T_{\alpha,l}^m + \left(\frac{\alpha+1}{2\alpha+1}\right)T_{\alpha+1,l}^m\right] - (l+m)T_{\alpha,l-1}^m \tag{14}$$

we find, for $l > m$,

$$T_{l+m+1,l}^m = \frac{1}{2}\left(\frac{l+m+1}{l-m}\right)\left(\frac{2l-1}{2l+2m+3}\right)T_{l+m,l-1}^m, \tag{15}$$

a formula relating the last non-null element of column l to the last non-null element of column $(l - 1)$. Equation (15) can thus be used recursively to generate all required initial values for backward recursion of Eq. (13), provided the last non-null element of the first column, $T_{2m+1,m}^m$, is known. We can derive a recursion formula for $T_{2m+1,m}^m$ if we let $m \Leftarrow m - 1$ and set $\alpha = 2m + 1$ in Eq. (6); combining the result with Eq. (15), we find

$$T_{2m+1,m}^m = -\left(\frac{m}{2}\right)\left[\frac{(2m-1)(2m+1)}{(4m+1)(4m+3)}\right]T_{2m-1,m-1}^{m-1}, \tag{16}$$

which can be started with $T_{1,0}^0 = 1/6$.

To initiate forward recursion of Eq. (13), we have already mentioned that we require the first four rows of the $\mathbf{T}^m$ matrix. Defining the linear combinations

$$U_{0,l}^m = T_{0,l}^m, \tag{17a}$$

$$U_{1,l}^m = T_{1,l}^m + T_{0,l}^m, \tag{17b}$$

$$U_{2,l}^m = T_{2,l}^m + 3T_{1,l}^m + 2T_{0,l}^m \tag{17c}$$

and

$$U^m_{3,l} = T^m_{3,l} + 5T^m_{2,l} + 9T^m_{1,l} + 5T^m_{0,l}, \tag{17d}$$

for $l = m, m+1, \ldots, L$, we can show, with the help of Eq. (4), that the $U^m_{\alpha,l}$, $\alpha = 0, \ldots, 3$, satisfy the recursion relation

$$(2 + \alpha + l + m)U^m_{\alpha,l} = \left[\frac{(l+m-1)(l+m)}{(l-m-1)(l-m)}\right](3 + \alpha - l + m)U^m_{\alpha,l-2}. \tag{18}$$

Clearly, we need $U^m_{\alpha,m}$ and $U^m_{\alpha,m+1}$, $\alpha = 0, \ldots, 3$, to start Eq. (18). We can deduce convenient formulas for these starting values directly from Eq. (4). For $\alpha = 0$, we find that $U^m_{0,m}$ and $U^m_{0,m+1}$ can be computed recursively from

$$U^m_{0,m+k} = \left[\frac{(2m-1+k)(2m+k)}{(2m+2+k)}\right]U^{m-1}_{0,m-1+k}, \tag{19}$$

where $k = 0$ or $k = 1$, and $U^0_{0,k} = 1/(2+k)$ for $k = 0$ or 1. For $\alpha = 1$, 2 and 3, we can express all required starting values in terms of $U^m_{0,m}$ and $U^m_{0,m+1}$ as

$$U^m_{1,m} = \left(\frac{2}{2m+1}\right)U^m_{0,m+1}, \tag{20a}$$

$$U^m_{1,m+1} = 2\left(\frac{2m+1}{m+2}\right)U^m_{0,m}, \tag{20b}$$

$$U^m_{2,m} = \left(\frac{6}{m+2}\right)U^m_{0,m}, \tag{20c}$$

$$U^m_{2,m+1} = \left(\frac{18}{2m+5}\right)U^m_{0,m+1}, \tag{20d}$$

$$U^m_{3,m} = \left[\frac{60}{(2m+1)(2m+5)}\right]U^m_{0,m+1} \tag{20e}$$

and

$$U^m_{3,m+1} = 40\left[\frac{2m+1}{(m+2)(m+3)}\right]U^m_{0,m}. \tag{20f}$$

Once $U^m_{\alpha,l}$, $\alpha = 0, \ldots, 3$ and $l = m, m+1, \ldots, L$, are computed, we can easily obtain the first four rows of the $\mathbf{T}^m$ matrix by inverting Eqs. (17). We find, for $l = m, m+1, \ldots, L$,

$$T^m_{0,l} = U^m_{0,l}, \tag{21a}$$

$$T^m_{1,l} = U^m_{1,l} - U^m_{0,l}, \tag{21b}$$

$$T^m_{2,l} = U^m_{2,l} - 3U^m_{1,l} + U^m_{0,l} \tag{21c}$$

and

$$T^m_{3,l} = U^m_{3,l} - 5U^m_{2,l} + 6U^m_{1,l} - U^m_{0,l}. \tag{21d}$$

To conclude this section, first we note that we may encounter singularities while using Eq. (13) in the forward direction. These singularities arise because the factor $(4 + \alpha - l + m)$ which appears in the denominator when Eq. (13) is used in the forward direction can be zero. Clearly, the problem occurs once for each of the columns of the $\mathbf{T}^m$ matrix where the condition $I^m_l \geqslant l - m$ is satisfied and can be avoided simply by using Eq. (5) to compute the elements that cannot be computed by Eq. (13). Second, it should be mentioned that the $T^m_{\alpha,l}$ integrals do approach very large values as $m \to \infty$. Consequently, in order to avoid computer overflows, we have used a special floating-point number representation[6] in our program that consists in using different memory allocations to store the mantissa and the base 10 exponent of each of the required $T^m_{\alpha,l}$. This way, avoidance of computer overflows in our program was easy to achieve although it implied a sensible increase in computational cost.

4. NUMERICAL IMPLEMENTATION AND CONCLUDING REMARKS

We have programmed and implemented our scheme for computing the $T^m_{\alpha,l}$ integrals on two computers: a CDC CYBER 170/750 and a CDC 4360. The program was written in the FORTRAN language and was implemented in single precision on the long word-length machine (CYBER 170/750) and double precision on the short word-length machine (CDC 4360).

In regard to the factors ϵ and δ discussed in Sec. 3, we elected to use $\epsilon = 3 \times 10^{-14}$ and $\delta = 3 \times 10^{-9}$ on the CYBER machine and $\epsilon = 3 \times 10^{-15}$ and $\delta = 3 \times 10^{-10}$ on the CDC 4360. We note that the magnitude of δ, the factor controlling the accuracy of the calculation, was selected in order to try to avoid, or at least minimize, the occurrence of warning messages associated with accuracy criterion violations at run time (see Sec. 3). With these choices of ϵ and δ, we did not observe any warning messages while running our program on the CDC 4360 for $\alpha = 0, 1, \ldots, L + m + 1$, $l = m, m + 1, \ldots, L$ and $m = 0, 1, \ldots, L$, where $L = 299$. On the CYBER, a similar calculation originated 13 warning messages; an analysis of the magnitudes of the deviations between the perturbed and the unperturbed results revealed that the least accurate of the elements responsible for these warning messages had an accuracy of 8 significant figures. Therefore, our CDC 4360 results can be regarded as 10-figure accurate while our CYBER results are on the borderline of the 8- and 9-figure accuracy levels. We should make it clear to the reader, however, that our computational scheme is not capable of providing results accurate to these accuracy levels for null or near-null $T^m_{\alpha,l}$ elements that have non-null neighbors.

As a way of increasing our confidence on the effectiveness of the proposed scheme, we also checked our results against reference results generated by Marinho[8] who used the *Mathematica* system[9] to perform the integral of Eq. (1) for selected values of α, l and m and to some results of a FORTRAN multiple-precision arithmetic package.[10] As the $T^m_{\alpha,l}$ are rational numbers, both classes of reference results are exact, providing a benchmark for the calculation. At this point, one might ask why the tools that we used to generate the reference results cannot be used to compute the required $T^m_{\alpha,l}$ on a routine basis. The answer to this question is simple: although these tools are relatively economical for small to moderate values of α and l, they become highly expensive when any of these indices is large and so a complete calculation of the required $T^m_{\alpha,l}$ integrals with these tools is not feasible in this case.

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