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A NEW QUADRATURE SCHEME FOR SOLVING AZIMUTHALLY DEPENDENT TRANSPORT PROBLEMS

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ABSTRACT

A quadrature scheme that is particularly well suited for solving azimuthally dependent transport problems with the ANISN code is introduced. A brief description of the fundamental problem in the constructive theory of orthogonal polynomials is provided. The implementation of the modified Chebyshev and the linear-factor modification algorithms for computing sets of recurrence coefficients that are used to generate the required quadratures is discussed in detail. While both algorithms are very effective and yield accurate quadrature nodes and weights, the linear-factor modification algorithm has the advantage of being about 20% faster than the modified Chebyshev algorithm.

1. INTRODUCTION

In a recent work [1] we reported an improved way of implementing the ANISN code [2] for solving transport problems with azimuthal dependence. When compared to a previous ANISN implementation for the same class of problems,[3] our procedure showed the following advantages: (i) simpler and faster treatment of the scattering term in the transport equation; (ii) preservation of particle balance for all of the Fourier component problems; and

(iii) more accurate treatment of external particle incidence. Here we present in detail our algorithms for generating a quadrature which is basic to our improved ANISN implementation.

We consider the problem defined by the transport equation

$$\mu\frac{\partial}{\partial x}\psi(x,\mu,\varphi)+\sigma_t\,\psi(x,\mu,\varphi)=\sigma_s\int_{-1}^{1}\int_{0}^{2\pi}p(\cos\Theta)\psi(x,\mu',\varphi')\mathrm{d}\varphi'\mathrm{d}\mu',\qquad(1)$$

where $\psi(x,\mu,\varphi)$ denotes the angular flux of particles for $x\in(0,a)$, $\mu\in[-1,1]$ and $\varphi\in[0,2\pi]$, and the boundary conditions

$$\psi(0,\mu,\varphi)=\pi\delta(\mu-\mu_0)\delta(\varphi-\varphi_0)$$
$$\psi(a,-\mu,\varphi)=0\qquad(2)$$

for $\mu\in(0,1]$ and $\varphi\in[0,2\pi]$. In addition, we consider that in Eq. (1) the scattering law $p(\cos\Theta)$, where Θ is the scattering angle, is expressed as a truncated Legendre polynomial expansion, viz.

$$p(\cos\Theta)=\frac{1}{4\pi}\sum_{l=0}^{L}\beta_l P_l(\cos\Theta),\qquad(3)$$

and that σ_t and σ_s are, respectively, the macroscopic total and scattering cross sections of the host medium.

2. BASIC FORMULATION

In our formulation, the problem expressed by Eqs. (1) and (2) is first split into an uncollided and a collided problem.[4] By using a Fourier decomposition[4] and the addition theorem for the Legendre polynomials,[5] the latter is subsequently reduced to a series of $(L+1)$ problems without azimuthal dependence that are defined, for $m=0,1,\dots,L$, by the transport equation

$$\mu\frac{\partial}{\partial x}\psi_c^m(x,\mu)+\sigma_t\,\psi_c^m(x,\mu)=\frac{\sigma_s}{2}\sum_{l=m}^{L}\beta_l P_l^m(\mu)\times\int_{-1}^{1}P_l^m(\mu')\psi_c^m(x,\mu')\mathrm{d}\mu'+Q^m(x,\mu)\qquad(4)$$

and the boundary conditions, for $\mu\in(0,1]$,

$$\psi_c^m(0,\mu)=\psi_c^m(a,-\mu)=0.\qquad(5)$$

We note that these problems are usually referred to as *Fourier component problems* in the literature, and that the source in Eq. (4) comes from the uncollided contribution and is given by

$$Q^m(x,\mu)=\frac{\sigma_s}{2}e^{-\sigma_t x/\mu_0}\sum_{l=m}^{L}\beta_l P_l^m(\mu)P_l^m(\mu_0).\qquad(6)$$

In addition, the *normalized* associated Legendre functions $P_l^m(\mu)$, for $l\geq m$, are defined as

$$P_l^m(\mu)=\left[\frac{(l-m)!}{(l+m)!}\right]^{1/2}(1-\mu^2)^{m/2}\frac{\mathrm{d}^m}{\mathrm{d}\mu^m}P_l(\mu)\qquad(7)$$

and satisfy the recurrence formula

$$(2l+1)\mu P_l^m(\mu)=[(l+1)^2-m^2]^{1/2}P_{l+1}^m(\mu)+(l^2-m^2)^{1/2}P_{l-1}^m(\mu)\qquad(8)$$

for $l=m,m+1,\dots$, with initial value

$$P_m^m(\mu)=\left[\frac{(2m-1)!!}{(2m)!!}\right]^{1/2}(1-\mu^2)^{m/2}.\qquad(9)$$

As shown in detail in our previous work,[1] once the problems defined by Eqs. (4) and (5) are solved for $m=0,1,\dots,L$, the collided contribution to the solution of our original problem is readily available in terms of the solutions to these problems as

$$\psi_c(x,\mu,\varphi)=\frac{1}{2}\sum_{m=0}^{L}(2-\delta_{0,m})\psi_c^m(x,\mu)\cos[m(\varphi-\varphi_0)].\qquad(10)$$

Thus, we summarize next our way[1] of implementing the ANISN code to solve the problems defined by Eqs. (4) and (5).

We start by using the transformation

$$\psi_c^m(x,\mu)=(1-\mu^2)^{m/2}F^m(x,\mu)\qquad(11)$$

and introducing the associated Legendre *polynomials*, for $l \geq m$,

$$D_l^m(\mu) = \left[\frac{(2m)!!}{(2m-1)!!}\right]^{1/2} \left[\frac{(l-m)!}{(l+m)!}\right]^{1/2} \frac{\mathrm{d}^m}{\mathrm{d}\mu^m} P_l(\mu), \tag{12}$$

normalized so that $D_m^m(\mu) = 1$, to reformulate the problem given by Eqs. (4) and (5) as

$$\mu \frac{\partial}{\partial x} F^m(x,\mu) + \sigma_t F^m(x,\mu) = \frac{\sigma_s}{2}\left[\frac{(2m-1)!!}{(2m)!!}\right] \times \sum_{l=m}^{L} \beta_l D_l^m(\mu) \int_{-1}^{1} (1-\mu'^2)^m D_l^m(\mu') F^m(x,\mu')\mathrm{d}\mu' + S^m(x,\mu), \tag{13}$$

where

$$S^m(x,\mu) = \frac{\sigma_s}{2}\left[\frac{(2m-1)!!}{(2m)!!}\right](1-\mu_0^2)^{m/2} e^{-\sigma_t x/\mu_0} \sum_{l=m}^{L} \beta_l D_l^m(\mu) D_l^m(\mu_0), \tag{14}$$

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

$$F^m(0,\mu) = F^m(a,-\mu) = 0. \tag{15}$$

On comparing Eq. (13) with the usual transport equation that is solved by the ANISN code,[2] we find that, aside from the replacement of the Legendre polynomials $P_l(\mu)$ by the more general associated Legendre polynomials $D_l^m(\mu)$, the scattering integral in Eq. (13) has the extra factor $(1-\mu'^2)^m$ as a weighting function. It is thus clear that if we use a numerical quadrature based on this weighting function to approximate the scattering integral in Eq. (13), then we can use the ANISN code with minor modifications to find a discrete ordinates solution to Eq. (13) subject to Eqs. (15). Moreover, as we intend to keep the advantage of using a double quadrature, i.e. a quadrature designed to integrate a function over the $(-1,0)$ and $(0,1)$ intervals separately, in order to represent better the angular-flux discontinuities that occur at the boundaries for $|\mu| \to 0$, we consider first the quadrature defined so that, for a polynomial $C(\xi)$ of degree $\leq 2n-1$, the formula

$$\int_0^1 (1-\xi^2)^m C(\xi)\mathrm{d}\xi = \sum_{i=1}^{n} \eta_i^m C(\xi_i^m) \tag{16}$$

is exact. Here ξ_i^m and η_i^m, $i = 1,2,\ldots,n$, are respectively the nodes and weights of the quadrature of order n for the problem with Fourier index m. Once these nodes and weights are determined, it is only necessary to consider them together with their counterparts for the half-interval $(-1,0)$, i.e. $\{-\xi_i^m\}$ and $\{\eta_i^m\}$, to find the nodes and weights of the quadrature of order $N = 2n$ for the full interval $(-1,1)$. As explained in the subsequent sections of this work, the construction of such quadrature sets is based upon the determination of the recurrence coefficients for the (monic) orthogonal polynomials generated by the weighting function $(1-\xi^2)^m$, $\xi \in (0,1)$. These coefficients are computed in this work by means of two different algorithms: the modified Chebyshev algorithm[6–9] and the linear-factor modification algorithm.[7,10]

3. CONSTRUCTIVE THEORY OF ORTHOGONAL POLYNOMIALS

To solve the so-called fundamental problem in the constructive theory of orthogonal polynomials,[6,7] we are given a positive measure $\mathrm{d}\tau(\xi)$ on the real line $\Re$ or, alternatively, the first $2n$ (finite) moments of that measure,

$$U_k = \int_{\Re} \xi^k \mathrm{d}\tau(\xi), \qquad k = 0,1,\ldots,2n-1, \tag{17}$$

with $U_0 > 0$, and we are required to find the unique set of orthogonal polynomials $\Pi_k(\xi) = \Pi_k(\xi;\mathrm{d}\tau)$, $k = 0,1,\ldots,n$, defined by

$$\Pi_k(\xi) = \xi^k + \text{lower degree terms},$$
$$\int_{\Re} \Pi_k(\xi)\Pi_l(\xi)\mathrm{d}\tau(\xi) \begin{cases} = 0 & \text{if } k \neq l, \\ > 0 & \text{if } k = l, \end{cases} \qquad 0 \leq k,l \leq n. \tag{18}$$

As these polynomials satisfy a three-term recurrence relation of the form

$$\Pi_{k+1}(\xi) = (\xi - \alpha_k)\Pi_k(\xi) - \beta_k \Pi_{k-1}(\xi), \qquad k = 0,1,\ldots,n-1, \tag{19}$$
$$\Pi_{-1}(\xi) = 0, \qquad \Pi_0(\xi) = 1,$$

where $\alpha_k = \alpha_k(\mathrm{d}\tau)$ and $\beta_k = \beta_k(\mathrm{d}\tau) > 0$ are real constants, the fundamental problem in the constructive theory of orthogonal polynomials can be stated in the following terms: given $d\tau(\xi)$ on $\Re$ and n, compute $\alpha_k(d\tau)$ and $\beta_k(d\tau)$ for $k = 0, 1, \ldots, n-1$. Following Gautschi,[6] we introduce the vector of recurrence coefficients

$$\boldsymbol{\rho} = [\alpha_0, \ldots, \alpha_{n-1}, \beta_0, \ldots, \beta_{n-1}]^{\mathrm{T}} \in \Re^{2n}, \tag{20}$$

and note that the fundamental problem stated in this way requires us to implement the map $\Sigma(\Re) \to \Re^{2n}$ defined by $d\tau \to \boldsymbol{\rho}$, where $\Sigma(\Re)$ is some appropriate measure space on $\Re$. Due to its infinite dimension, such a map cannot be handled on a computer. An alternative is to depart not from $d\tau$, but from its first $2n$ moments given by Eq. (17).

To be more general, we assume that we are given the first $2n$ *modified* moments of $d\tau$,

$$M_k = \int_{\Re} \mathcal{P}_k(\xi) d\tau(\xi), \qquad k = 0, 1, \ldots, 2n-1, \tag{21}$$

where $\{\mathcal{P}_k(\xi)\}$ is a system of polynomials that satisfies

$$\begin{aligned} &\mathcal{P}_{k+1}(\xi) = (\xi - a_k)\mathcal{P}_k(\xi) - b_k \mathcal{P}_{k-1}(\xi), \qquad k = 0, 1, \ldots, 2n-2, \\ &\mathcal{P}_{-1}(\xi) = 0, \qquad \mathcal{P}_0(\xi) = 1, \end{aligned} \tag{22}$$

with known coefficients $\{a_k\}$ and $\{b_k\}$. The fundamental problem can thus be restated in the following terms: given the first $2n$ modified moments of $d\tau$ defined by Eq. (21), compute $\alpha_k(d\tau)$ and $\beta_k(d\tau)$ for $k = 0, 1, \ldots, n-1$. Defining the vector of modified moments

$$\mathbf{M} = [M_0, M_1, \ldots, M_{2n-1}]^{\mathrm{T}} \in \Re^{2n}, \tag{23}$$

we now have to implement the finite-dimensional (nonlinear) map

$$K_n : \Re^{2n} \to \Re^{2n} \qquad \mathbf{M} \to \boldsymbol{\rho}. \tag{24}$$

In the case where $a_k = b_k = 0$ in Eq. (22), which is equivalent to $\mathcal{P}_k(\xi) = \xi^k$ and $M_k = U_k$, the map K_n can be written in determinantal form. However, this map becomes highly ill conditioned for n large, and is therefore of little practical use.

4. THE MODIFIED CHEBYSHEV ALGORITHM

The ill conditioning of the map K_n can be resolved through the utilization of the modified Chebyshev algorithm,[6–9] in which case the desired recurrence coefficients $\alpha_k(d\tau)$ and $\beta_k(d\tau)$, $k = 0, 1, \ldots, n-1$, of the polynomials $\Pi_k(\xi; d\tau)$ are obtained in terms of the *mixed* moments

$$\tau_{k,l} = \int_{\Re} \Pi_k(\xi)\Gamma_l(\xi) d\tau(\xi), \qquad k \le l. \tag{25}$$

Here the auxiliary polynomials $\Gamma_l(\xi)$ are orthogonal with respect to a given measure $ds(\xi)$ and their recurrence coefficients $\{a_l\}$ and $\{b_l\}$ are considered to be known. We note that $\tau_{k,l} = 0$ if $k > l$ in Eq. (25), by orthogonality. In addition, we have

$$\begin{aligned} &\tau_{-1,l} = 0, \qquad l = 1, 2, \ldots, 2n-2, \\ &\tau_{0,l} = M_l, \qquad l = 0, 1, \ldots, 2n-1, \\ &\alpha_0 = a_0 + M_1/M_0, \qquad \beta_0 = M_0, \end{aligned} \tag{26}$$

which are used to initialize the algorithm. Once this is done, the computation of the $\tau_{k,l}$ moments and the α_k and β_k coefficients is carried out by using the following formulas cyclically for $k = 1, 2, \ldots, n-1$:

$$\begin{aligned} &\tau_{k,l} = \tau_{k-1,l+1} - (\alpha_{k-1} - a_l)\tau_{k-1,l} - \beta_{k-1}\tau_{k-2,l} + b_l \tau_{k-1,l-1}, \\ &\qquad\qquad l = k, k+1, \ldots, 2n-k-1, \\ &\alpha_k = a_k + \frac{\tau_{k,k+1}}{\tau_{k,k}} - \frac{\tau_{k-1,k}}{\tau_{k-1,k-1}}, \\ &\beta_k = \frac{\tau_{k,k}}{\tau_{k-1,k-1}}. \end{aligned} \tag{27}$$

Our specific problem can be put in the framework of the general theory by denoting our desired polynomials for the Fourier index m as $R_k^m(\xi)$, conveniently choosing $R_l^{m-1}(\xi)$ as the auxiliary polynomials, and considering that the measure is given by $d\tau(\xi) = (1 - \xi^2)^m d\xi$ for $\xi \in [0, 1]$ and $d\tau(\xi) = 0$ for

$\xi \notin [0,1]$. We thus find that Eq. (25) becomes

$$\tau_{k,l}^m = \int_0^1 R_k^m(\xi) R_l^{m-1}(\xi)(1-\xi^2)^m \mathrm{d}\xi, \qquad k \le l. \tag{28}$$

With this convenient choice of the auxiliary polynomials, we can easily show that $\tau_{k,l}^m = 0$, $l > k+2$, and so our set of formulas for computing the desired recurrence coefficients, for any $m = 1, 2, \ldots, L$, becomes

$$\begin{aligned} &\tau_{-1,1}^m = 0, \\ &\tau_{0,l}^m = M_l^m, \qquad l = 0,1,2, \\ &\alpha_0^m = \alpha_0^{m-1} + M_1^m/M_0^m, \qquad \beta_0^m = M_0^m, \end{aligned} \tag{29}$$

and, for $k = 1, 2 \ldots, n-1+2(L-m)$,

$$\begin{aligned} \tau_{k,k}^m &= \tau_{k-1,k+1}^m - (\alpha_{k-1}^m - \alpha_k^{m-1})\tau_{k-1,k}^m - \beta_{k-1}^m \tau_{k-2,k}^m + \beta_k^{m-1}\tau_{k-1,k-1}^m, \\ \tau_{k,k+1}^m &= -(\alpha_{k-1}^m - \alpha_{k+1}^{m-1})\tau_{k-1,k+1}^m + \beta_{k+1}^{m-1}\tau_{k-1,k}^m, \\ \tau_{k,k+2}^m &= \beta_{k+2}^{m-1}\tau_{k-1,k+1}^m, \\ \alpha_k^m &= \alpha_k^{m-1} + \frac{\tau_{k,k+1}^m}{\tau_{k,k}^m} - \frac{\tau_{k-1,k}^m}{\tau_{k-1,k-1}^m}, \\ \beta_k^m &= \frac{\tau_{k,k}^m}{\tau_{k-1,k-1}^m}, \end{aligned} \tag{30}$$

where we observe that the coefficients of the $(m-1)$ family are utilized to compute the coefficients of the m family, and that it is necessary to compute two extra values for the $(m-1)$ family in order to determine all of the required values for the m family. As will be shown shortly, the $m = 0$ family of orthogonal polynomials can be easily determined, and so the algorithm can be used successively for $m = 1, 2, \ldots, L$ to obtain all of the required polynomial families. Finally, the modified moments that serve to initialize the calculation for any $m \ge 1$ are defined in our case by

$$M_l^m = \int_0^1 R_l^{m-1}(\xi)(1-\xi^2)^m \mathrm{d}\xi, \qquad l = 0,1,2. \tag{31}$$

As mentioned above, we need to determine the family of orthogonal polynomials for $m = 0$ in order to initiate the application of our modified Chebyshev algorithm expressed by Eqs. (29) and (30). By noting that for $m = 0$ the weighting function reduces to unity in the interval $[0,1]$ and vanishes outside of this interval, we conclude that $R_l^0(\xi)$, the $(l+1)$-th element of the desired family of orthogonal polynomials for $m = 0$, is proportional to $P_l(2\xi - 1)$, the shifted Legendre polynomial.[11] By using the explicit formula[12]

$$P_l(2\xi - 1) = \sum_{k=0}^{l} (-1)^{l+k} \frac{(l+k)!}{(l-k)!(k!)^2} \xi^k, \tag{32}$$

we find that

$$R_l^0(\xi) = \frac{(l!)^2}{(2l)!} P_l(2\xi - 1), \tag{33}$$

where the fraction $(l!)^2/(2l)!$ is a normalization factor used to reduce to unity the coefficient of the highest power in $P_l(2\xi - 1)$. By using Eq. (33) and the recurrence formula for the shifted Legendre polynomials,[11] we find that the $R_l^0(\xi)$ polynomials must satisfy the recurrence formula

$$R_{l+1}^0(\xi) = (\xi - \tfrac{1}{2})R_l^0(\xi) - \frac{l^2}{4(2l-1)(2l+1)} R_{l-1}^0(\xi). \tag{34}$$

Thus, by comparing Eqs. (19) and (34), we find that the coefficients α_k^0 and β_k^0 required to initiate the application of our algorithm are given by

$$\alpha_k^0 = \frac{1}{2}, \qquad \beta_k^0 = \delta_{0,k} + \frac{k^2}{4(4k^2-1)}, \qquad k = 0, 1, \ldots, n-1+2L, \tag{35}$$

where the Kronecker delta was introduced so that $\beta_0^0 = \int_0^1 \mathrm{d}\xi = 1$ [note that β_0^0 is in fact arbitrary, since $R_{-1}^0(\xi) = 0$].

Turning now our attention to the determination of the M_l^m moments that are defined by Eq. (31) and required in Eqs. (29) for $m = 1, 2, \ldots, L$, we note that by using the initial values $R_{-1}^m(\xi) = 0$ and $R_0^m(\xi) = 1$ along with Eq. (19)

for $k = 0$ and $k = 1$ we first obtain, since $\Pi_k(\xi) \equiv R_k^m(\xi)$,

$$R_1^m(\xi) = \xi - \alpha_0^m,$$
$$R_2^m(\xi) = (\xi - \alpha_1^m)R_1^m(\xi) - \beta_1^m R_0^m(\xi). \qquad (36)$$

Finally, we can determine the required M_l^m moments by explicitly integrating $R_0^m(\xi)$, $R_1^m(\xi)$ and $R_2^m(\xi)$. We find

$$M_0^m = \int_0^1 (1-\xi^2)^m \mathrm{d}\xi = \left(\frac{2m}{2m+1}\right) M_0^{m-1}, \qquad M_0^0 = 1,$$
$$M_1^m = \int_0^1 R_1^{m-1}(\xi)(1-\xi^2)^m \mathrm{d}\xi = \int_0^1 (\xi - \alpha_0^{m-1})(1-\xi^2)^m \mathrm{d}\xi$$
$$= \left(\frac{1}{2m+2}\right) - \alpha_0^{m-1} M_0^m,$$
$$M_2^m = \int_0^1 R_2^{m-1}(\xi)(1-\xi^2)^m \mathrm{d}\xi$$
$$= \int_0^1 (\xi - \alpha_1^{m-1}) R_1^{m-1}(\xi)(1-\xi^2)^m \mathrm{d}\xi - \beta_1^{m-1} \int_0^1 (1-\xi^2)^m \mathrm{d}\xi$$
$$= \left[\left(\frac{1}{2m+3}\right) - \left(\alpha_0^{m-1}\right)^2 - \beta_1^{m-1}\right] M_0^m - \left[\alpha_0^{m-1} + \alpha_1^{m-1}\right] M_1^m. \qquad (37)$$

5. THE LINEAR-FACTOR MODIFICATION ALGORITHM

In the constructive theory of orthogonal polynomials, the following problem may arise: given a positive measure on $\Re$, expressed as $\mathrm{d}\tau$ times a polynomial, construct the orthogonal polynomials for this measure in terms of those for the measure $\mathrm{d}\tau$. An expression for the new (modified) polynomials is provided by the classical formula of Christoffel,[13] but the result is expressed in determinantal form. From a computational point of view, it is more practical to obtain the recurrence coefficients $\{\alpha_k\}$ and $\{\beta_k\}$ for the modified polynomials in terms of those for the original polynomials, $\{a_k\}$ and $\{b_k\}$, by using the linear-factor modification algorithm.[7,10]

A more complete statement of the problem is the following: given the orthogonal polynomials $\{P_n(\xi)\}$ associated with a weighting function $w(\xi)$ on the interval (a, b) and the polynomial $X(\xi)$ of degree l, nonnegative on this interval, construct the orthogonal polynomials $\{Q_n(\xi)\}$ associated with the weighting function $X(\xi)w(\xi)$ on the same interval. Because a polynomial can always be factored as a product of linear factors, it is sufficient to consider the polynomial $X(\xi)$ as being of degree $l = 1$. The most general case can then be treated as a succession of linear cases. For $l = 1$, the Christoffel theorem provides an expression for the modified polynomial $Q_n(\xi)$ in the form

$$Q_n(\xi)X(\xi) = K_n(s) \begin{vmatrix} P_n(\xi) & P_{n+1}(\xi) \\ P_n(s) & P_{n+1}(s) \end{vmatrix} \qquad (38)$$

or, more explicitly,

$$Q_n(\xi)(\xi - s) = K_n(s)[P_n(\xi)P_{n+1}(s) - P_{n+1}(\xi)P_n(s)], \qquad (39)$$

where $s \le a$ is the root of the polynomial $X(\xi)$ (the modification needed to treat the case $s \ge b$ will be presented at the end of this section) and $K_n(s)$ is a normalization constant, to be determined so that the coefficient of the highest power in $Q_n(\xi)$ be unity. In addition, it is assumed that the polynomial $P_j(\xi)$ satisfies the three-term recurrence relation

$$P_{j+1}(\xi) = (\xi - a_j)P_j(\xi) - b_j P_{j-1}(\xi), \qquad j = 0, 1, \dots, \qquad (40)$$
$$P_{-1}(\xi) = 0, \qquad P_0(\xi) = 1,$$

with known coefficients $\{a_j\}$ and $\{b_j\}$.

Due to the difficulty in finding a complete, step-by-step derivation of this algorithm in the literature, we present here such a derivation. Initially, we subtract Eq. (40) multiplied by $P_j(s)$ from the equation that is obtained by changing ξ to s in Eq. (40) and multiplying the result by $P_j(\xi)$. We obtain

$$b_j[P_{j-1}(\xi)P_j(s) - P_j(\xi)P_{j-1}(s)]$$
$$- [P_j(\xi)P_{j+1}(s) - P_{j+1}(\xi)P_j(s)] = (\xi - s)P_j(\xi)P_j(s). \qquad (41)$$

Next, we multiply Eq. (41) by $\prod_{k=j}^{n-1} b_{k+1}$ and add the equations obtained from using the resulting equation for $j = 0, 1, \ldots, n$ to get

$$P_n(\xi)P_{n+1}(s) - P_{n+1}(\xi)P_n(s) = -(\xi - s)\sum_{j=0}^{n}\left(\prod_{k=j}^{n-1} b_{k+1}\right) P_j(\xi)P_j(s). \quad (42)$$

Considering Eqs. (39) and (42), we conclude that the desired polynomials can be expressed in the form

$$Q_n(\xi) = \frac{1}{P_n(s)}\sum_{j=0}^{n}\left(\prod_{k=j}^{n-1} b_{k+1}\right) P_j(\xi)P_j(s), \quad (43)$$

where we took $K_n(s) = -1/P_n(s)$ in order to reduce to unity the coefficient of the highest power in $Q_n(\xi)$. Clearly, these polynomials must also satisfy a three-term recurrence relation of the form

$$Q_{j+1}(\xi) = (\xi - \alpha_j)Q_j(\xi) - \beta_j Q_{j-1}(\xi). \quad (44)$$

Now, manipulating Eq. (43) we obtain the following expressions:

$$Q_n(\xi) = b_n \frac{P_{n-1}(s)}{P_n(s)} Q_{n-1}(\xi) + P_n(\xi) \quad (45)$$

and

$$Q_{n+1}(\xi) = b_{n+1}\frac{P_n(s)}{P_{n+1}(s)} Q_n(\xi) + P_{n+1}(\xi). \quad (46)$$

The result of adding Eqs. (45) and (46), after being multiplied, respectively, by $P_{n+1}(s)$ and $-P_n(s)$, is

$$Q_{n+1}(\xi) = \left[\xi - s + \frac{P_{n+1}(s)}{P_n(s)} + b_{n+1}\frac{P_n(s)}{P_{n+1}(s)}\right] Q_n(\xi) - b_n \frac{P_{n+1}(s)P_{n-1}(s)}{[P_n(s)]^2} Q_{n-1}(\xi) \quad (47)$$

or

$$Q_{n+1}(\xi) = (\xi - s - q_n - e_n)Q_n(\xi) - (e_{n-1}q_n)Q_{n-1}(\xi), \quad (48)$$

where

$$q_n = -\frac{P_{n+1}(s)}{P_n(s)}, \qquad e_n = -b_{n+1}\frac{P_n(s)}{P_{n+1}(s)} = \frac{b_{n+1}}{q_n}, \qquad n \geq 0. \quad (49)$$

Comparing Eqs. (44) and (48), we finally obtain the recurrence coefficients for the modified polynomials in terms of those for the original polynomials, for $k = 0, 1, \ldots, n-1$:

$$\alpha_k = s + q_k + e_k, \qquad \beta_k = \begin{cases} q_0 b_0 & \text{if } k = 0, \\ q_k e_{k-1} & \text{if } k > 0, \end{cases} \quad (50)$$

where $q_k = a_k - e_{k-1} - s$ and $e_k = b_{k+1}/q_k$, with $e_{-1} = 0$.

In order to apply this algorithm to our specific problem, we consider (as in the previous section) that the coefficients for the $(m-1)$ family are available and can be used to calculate the coefficients for the m family. The basic idea here is to factor our weighting function as $(1-\xi)(1+\xi)(1-\xi^2)^{m-1}$ and carry out, for each m, the calculation of the desired recurrence coefficients in two steps: in the first, we consider the modification introduced by the factor $(1+\xi)$ into the $(m-1)$ family and, in the second, the modification by the factor $(1-\xi)$ into the result of the first step. Hence, considering $m > 0$, the equations resulting from the modification by $(1+\xi)$ are given, for $k = 0, 1, \ldots, n + 2(L-m)$, by

$$\begin{aligned} q_k^{m-1/2} &= \alpha_k^{m-1} - e_{k-1}^{m-1/2} + 1, \\ e_k^{m-1/2} &= \beta_{k+1}^{m-1}/q_k^{m-1/2}, \\ \alpha_k^{m-1/2} &= -1 + q_k^{m-1/2} + e_k^{m-1/2}, \\ \beta_k^{m-1/2} &= \begin{cases} q_0^{m-1/2}\beta_0^{m-1} & \text{if } k = 0, \\ q_k^{m-1/2}e_{k-1}^{m-1/2} & \text{if } k > 0, \end{cases} \end{aligned} \quad (51)$$

with $e_{-1}^{m-1/2} = 0$ and where we use the superscript $(m-1/2)$ to identify the parameters obtained from the first step of modification applied to the $(m-1)$ family. Finally, the equations resulting from the modification by $(1-\xi)$ are given, for $k = 0, 1, \ldots, n - 1 + 2(L-m)$, by

$$\begin{aligned} q_k^m &= \alpha_k^{m-1/2} - e_{k-1}^m - 1, \\ e_k^m &= \beta_{k+1}^{m-1/2}/q_k^m, \end{aligned}$$

$$\alpha_k^m = 1 + q_k^m + e_k^m, \qquad \beta_k^m = \begin{cases} |q_0^m|\beta_0^{m-1/2} & \text{if } k = 0, \\ q_k^m e_{k-1}^m & \text{if } k > 0, \end{cases} \tag{52}$$

with $e_{-1}^m = 0$. Noting the upper limits of k for which Eqs. (51) and (52) are used, we can clearly see that two extra values of all parameters are needed for $(m-1)$ in comparison to the number of parameters needed for m. In addition, we note that the modification by $(1-\xi)$ involves a sign change in the algorithm presented at the beginning of this section [instead of $\xi - s$, we must consider $s - \xi$ in Eq. (39)]. We can demonstrate that the general algorithm given by Eq. (50) can still be employed in this case, provided q_0 is replaced by $|q_0|$ in the expression for β_k, as done in Eq. (52).

6. QUADRATURE GENERATION

Once the coefficients $\{\alpha_k^m\}$ and $\{\beta_k^m\}$ are obtained with the modified Chebyshev algorithm [Equations (29), (30), (35) and (37)] or the linear-factor modification algorithm [Equations (35), (51) and (52)], the desired quadrature nodes $\{\xi_i^m\}$ and weights $\{\eta_i^m\}$ can be readily computed. By considering the $n \times n$ Jacobi matrix[6,7,14,15]

$$\mathbf{J}_n^m = \begin{pmatrix} \alpha_0^m & \sqrt{\beta_1^m} & & & & \\ \sqrt{\beta_1^m} & \alpha_1^m & \sqrt{\beta_2^m} & & & \\ & \sqrt{\beta_2^m} & \alpha_2^m & \sqrt{\beta_3^m} & & \\ & & \ddots & \ddots & \ddots & \\ & & & \sqrt{\beta_{n-2}^m} & \alpha_{n-2}^m & \sqrt{\beta_{n-1}^m} \\ & & & & \sqrt{\beta_{n-1}^m} & \alpha_{n-1}^m \end{pmatrix}, \tag{53}$$

whose characteristic polynomial is $R_n^m(\xi)$, i.e.

$$\det(\xi \mathbf{I}_n - \mathbf{J}_n^m) = R_n^m(\xi), \tag{54}$$

we find that we can obtain the nodes $\{\xi_i^m\}$ as the eigenvalues of $\mathbf{J}_n^m$. In addition, to each node ξ_i^m there corresponds a weight η_i^m given by

$$\eta_i^m = M_0^m u_{i,1}^2, \tag{55}$$

where $u_{i,1}$ is the first component of $\mathbf{u}_i$, the i-th normalized eigenvector of $\mathbf{J}_n^m$, i.e.

$$\mathbf{J}_n^m \mathbf{u}_i = \xi_i^m \mathbf{u}_i, \qquad \mathbf{u}_i^{\mathrm{T}} \mathbf{u}_i = 1, \tag{56}$$

and M_0^m can be computed with the help of the first of Eqs. (37). These calculations were performed with subroutine *Imtql3*, which is a modified version[16] of subroutine *Imtql2* of the EISPACK package.[17] The execution time of subroutine *Imtql3*, which computes only the first components of the eigenvectors and the eigenvalues of a symmetric tridiagonal matrix, is almost two orders of magnitude smaller than the execution time of subroutine *Imtql2*, thus providing considerable savings in computer time.

7. ALGORITHM COMPARISON AND CONCLUDING REMARKS

The accuracy of the generated nodes and weights was verified by utilizing the property of exact integration (except for computer rounding errors) of a polynomial of degree up to $(2n-1)$ by a quadrature of order n. We compared the results of the Gaussian integration of the moments

$$C_k^m = \int_0^1 (1-\xi^2)^m \xi^k d\xi, \tag{57}$$

which can be expressed exactly for $k = 0, 1, \ldots, 2n-1$ as

$$C_k^m = \sum_{i=1}^{n} \eta_i^m (\xi_i^m)^k, \tag{58}$$

with the analytical result

$$C_k^m = \frac{(k-1)!!(2m)!!}{(2m+k+1)!!}. \tag{59}$$

We note that, for computational purposes, instead of using Eq. (59) we used the recurrence relation, for $k \geq 2$,

$$C_k^m = \left(\frac{k-1}{2m+k+1}\right) C_{k-2}^m \tag{60}$$

TABLE 1
Nodes and Weights for a Quadrature of Order 10
and Four Selected Values of the Fourier Index

$\{\xi_i^5\}$	$\{\eta_i^5\}$	$\{\xi_i^{10}\}$	$\{\eta_i^{10}\}$
0.104364902105(−1)	0.266239257815(−1)	0.894415910241(−2)	0.228000545579(−1)
0.537587935496(1)	0.584313463887(−1)	0.459890162264(−1)	0.495545140705(−1)
0.127111525990	0.795659452023(−1)	0.108509805636	0.652778768670(−1)
0.224007379138	0.821203861804(−1)	0.191009770886	0.624332452827(−1)
0.337054536944	0.649038867646(−1)	0.287698810951	0.429667417654(−1)
0.458782735546	0.379318854966(−1)	0.393204107334	0.201892477866(−1)
0.582056613532	0.153936727634(1)	0.502792966039	0.597913731123(−2)
0.700303287396	0.390740998424(−2)	0.612428557957	0.985793687756(−3)
0.807732700247	0.509054815765(−3)	0.718939838892	0.722102640453(−4)
0.899888546656	0.208560304694(−4)	0.821072247181	0.136197943731(−5)
$\{\xi_i^{20}\}$	$\{\eta_i^{20}\}$	$\{\xi_i^{40}\}$	$\{\eta_i^{40}\}$
0.722597514652(−2)	0.184071644070(−1)	0.554961539332(−2)	0.141292566568(−1)
0.370915837184(−1)	0.396404555347(−1)	0.284501194516(−1)	0.302157751663(−1)
0.873458199099(−1)	0.506281384254(−1)	0.668991233590(−1)	0.377043530089(1)
0.153606750577	0.451546141760(1)	0.117570622022	0.319297038321(−1)
0.231615876678	0.274286431080(−1)	0.177439929272	0.177004922835(−1)
0.317813221429	0.106178405713(−1)	0.244226715957	0.595398175116(−2)
0.409452183979	0.238563017396(−2)	0.316464518035	0.109651424785(−2)
0.504618490562	0.270397335753(−3)	0.393543961636	0.949526377366(−4)
0.602510841271	0.120292714371(−4)	0.476104808052	0.294728637682(−5)
0.705191168410	0.114749742131(−6)	0.568198777205	0.170332337401(−7)

and the initial values, for $m \geq 1$,

$$C_0^m = \left(\frac{2m}{2m+1}\right) C_0^{m-1}, \tag{61}$$

with $C_0^0 = 1$, and, for $m \geq 0$,

$$C_1^m = \left(\frac{1}{2m+2}\right). \tag{62}$$

Although both algorithms proved to be very robust and yielded results of comparable accuracy for the required quadrature nodes and weights (basically

12 digits of accuracy in 16-digit computations, for quadratures of order up to 300), we found that the linear-factor modification algorithm has the advantage of being about 20% more efficient in terms of computer execution time than the modified Chebyshev algorithm. In Table 1, we provide a few sample results for quadrature nodes and weights that can be used to check independent implementations of these algorithms.

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Kinetic Theory of Atoms and Photon
An Application to the Milne–Chandr

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Abstract. We consider a kinetic model describing the i
with two internal energy levels. Using the moment equ
Next, we provide the existence and uniqueness theorer

1. Introduction In a recent paper [RSM], Ross
for the study of two-level atoms and monochroma
allows a good description of the problem, namel
one side, and interaction between gas and radia
a modelling is that, under thermodynamical equi
selfconsistently, without resorting to additional hy
An interesting application for the above kinetic
A slab is filled with a gas, illuminated from one
within the slab, of radiation field, excited atom d
In this report, after a brief description of the m
the Milne–Chandrasekhar problem and state exis
partial differential equations. In [MPR], we provi
stationary problem, as well as numerical solution

2. The Kinetic Model

Consider the following physical system:

(a) A gas of atoms A of mass m endowed with
what follows we will denote by A_1 and A_2,
and excited levels).

(b) A radiation field of photons p at a fixed fre