Pergamon
www.elsevier.com/locate/pnucene

Progress in Nuclear Energy, Vol. 35, No. 3–4, pp. 249–273, 1999

0149-1970/99/$ - see front matter

PII: S0149-1970(99)00018-9

THE APPLICATION OF NONCLASSICAL ORTHOGONAL POLYNOMIALS IN PARTICLE TRANSPORT THEORY

R. D. M. GARCIA

Centro Técnico Aeroespacial, Instituto de Estudos Avançados
12231-970 São José dos Campos, SP, Brazil

Abstract—In this work, the fundamentals of the constructive theory of orthogonal polynomials and their applications are reviewed. The review provides a basis for a subsequent discussion of transport-theory applications of nonclassical orthogonal polynomials that includes solutions to azimuthally-dependent transport problems, chemical kinetics problems, Fokker-Planck equations with nonlinear coefficients, and the problem of neutral particle transport in ducts.

1. INTRODUCTION

The analytical theory of orthogonal polynomials has been deeply investigated since the middle of the last century (Chebyshev, 1859; Christoffel, 1858; 1877; Darboux, 1878; Stieltjes, 1884), and can now be considered a well-established theory (Shohat, 1934; Szegö, 1939; Erdélyi *et al.*, 1953; Freud, 1971; Chihara, 1978).

Along the years, *classical* orthogonal polynomials have been applied in several disciplines: mathematics, physics, chemistry, statistics, electrical engineering, and many others. *Nonclassical* orthogonal polynomials, on the other hand, have not been widely used, mainly because their supporting theory does not share the close relationship with the theory of the fundamental differential equations of mathematical physics that is typical of the theory of classical polynomials and also because they are not so easy to generate, numerically speaking. However, the latter difficulty is much less severe today than it was 30 years ago: recent advances in the constructive theory of orthogonal polynomials have resulted in the development of accurate and efficient algorithms for generating nonclassical orthogonal polynomials. Consequently, the range of applications of these polynomials has expanded and they are now being applied in new fields of study, including particle transport theory.

The outline of this paper is as follows. In Section 2, the current status of the constructive theory of orthogonal polynomials is summarized. General applications of the theory are briefly discussed in Section 3 and various transport-theory applications of nonclassical orthogonal polynomials that have been reported in the literature are presented and discussed in Section 4. Finally, Section 5 consists of our concluding remarks.

2. THE CONSTRUCTIVE THEORY OF ORTHOGONAL POLYNOMIALS

2.1. The Fundamental Problem

The fundamental problem in the constructive theory of general orthogonal polynomials can be formulated in the following way (Gautschi, 1985). We are given a nonnegative measure $\mathrm{d}\tau(\xi)$ on the real line $\Re$ and the first $2n$ moments

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

which are assumed to be finite. We are required to find the unique set of monic orthogonal polynomials $\{\Pi_k(\xi),\ k = 0, 1, \dots, n\}$ (i.e. the set of orthogonal polynomials normalized so that the coefficient of the highest power in each of its elements is unity) that satisfy the orthogonality property

$$\int_{\Re} \Pi_k(\xi)\Pi_l(\xi)\mathrm{d}\tau(\xi) = N_k \delta_{k,l}, \qquad 0 \le k, l \le n, \tag{2}$$

and a three-term recurrence relation of the form

$$\Pi_{k+1}(\xi) = (\xi - \alpha_k)\Pi_k(\xi) - \beta_k \Pi_{k-1}(\xi), \qquad k = 0, 1, \dots, n-1, \tag{3}$$

with initial values $\Pi_{-1}(\xi) = 0$ and $\Pi_0(\xi) = 1$, for the indicated values of k and l. It is clear that the task of constructing the first $n+1$ polynomials $\{\Pi_k(\xi)\}$ can be considered accomplished once the coefficients α_k and β_k in Eq. (3) are known for $k = 0, 1, \dots, n-1$. Strictly speaking, the coefficient β_0 is not required in Eq. (3), and thus it can be chosen arbitrarily; however, as pointed out by Gautschi (1982a, 1985), it is convenient to choose

$$\beta_0 = \int_{\Re} \mathrm{d}\tau(\xi). \tag{4}$$

One of the advantages of this choice of β_0 is that the normalization constant in Eq. (2) can be expressed by the simple formula (Gautschi, 1982a)

$$N_k = \beta_0 \beta_1 \dots \beta_k. \tag{5}$$

At this point, we note that there are other ways of constructing orthogonal polynomials, the most traditional of which is based on the determination of the coefficients of their representations in terms of powers (Stroud and Secrest, 1966). However, as discussed in detail by Gautschi (1982a), there are several reasons why the approach based on the recurrence coefficients $\{\alpha_k\}$ and $\{\beta_k\}$ should be favored over the others.

If we now introduce (Gautschi, 1985) the vector of moments

$$\boldsymbol{\mu} = [\mu_0, \mu_1, \dots, \mu_{2n-1}]^T \tag{6}$$

and the vector of recurrence coefficients

$$\boldsymbol{\rho} = [\alpha_0, \alpha_1, \dots, \alpha_{n-1}, \beta_0, \beta_1, \dots, \beta_{n-1}]^T, \tag{7}$$

we can see that the fundamental problem requires us to implement the map

$$M_n : \Re^{2n} \to \Re^{2n} \qquad \boldsymbol{\mu} \to \boldsymbol{\rho}. \tag{8}$$

This map can be easily implemented by means of a procedure known as the Chebyshev algorithm (Gautschi, 1982a), but its use in practice is limited to small values of n, because the condition number of the map grows exponentially with n (Gautschi, 1968a; 1978), and the procedure becomes numerically unstable as n increases. An alternative is to depart not from the ordinary moments μ_k defined by Eq. (1) but from the *modified* moments

$$m_k = \int_{\Re} \mathcal{P}_k(\xi)\mathrm{d}\tau(\xi), \qquad k = 0, 1, \ldots, 2n-1, \tag{9}$$

where $\{\mathcal{P}_k(\xi)\}$ is a system of monic polynomials that satisfies the three-term recurrence relation

$$\mathcal{P}_{k+1}(\xi) = (\xi - a_k)\mathcal{P}_k(\xi) - b_k\mathcal{P}_{k-1}(\xi), \qquad k = 0, 1, \ldots, 2n-2, \tag{10}$$

with known coefficients $\{a_k\}$ and $\{b_k\}$ and initial values $\mathcal{P}_{-1}(\xi) = 0$ and $\mathcal{P}_0(\xi) = 1$. A judicious choice of the $\mathcal{P}$-polynomials—usually a set of orthogonal polynomials—can greatly improve the numerical condition of the problem. However, before elaborating on this point, we illustrate our presentation by giving some examples of systems of orthogonal polynomials.

2.2. Examples of Systems of Orthogonal Polynomials

We begin with a few examples of classical orthogonal polynomials (Erdélyi *et al.*, 1953; Hochstrasser, 1964). The simplest case is perhaps that of the uniform measure on $[-1, 1]$,

$$\mathrm{d}\tau(\xi) = \begin{cases} \mathrm{d}\xi, & \xi \in [-1, 1], \\ 0, & \text{otherwise}, \end{cases} \tag{11}$$

which is associated with the Legendre polynomials $\{P_k(\xi)\}$. As these polynomials satisfy the recurrence relation

$$P_{k+1}(\xi) = \frac{2k+1}{k+1}\,\xi P_k(\xi) - \frac{k}{k+1}P_{k-1}(\xi), \qquad k \geq 0, \tag{12}$$

with initial value $P_0(\xi) = 1$, and the coefficients of their highest powers are given by $(2k-1)!!/k!$ for $k \geq 0$, it is clear that the corresponding set of monic orthogonal polynomials has elements

$$\Pi_k(\xi) = \frac{k!}{(2k-1)!!}P_k(\xi), \qquad k \geq 0. \tag{13}$$

In addition, using Eqs. (12) and (13), we can readily show that the recurrence coefficients in Eq. (3) are given in this case by $\alpha_k = 0$ and $\beta_k = 2\delta_{0,k} + k^2/(4k^2-1)$, where the term with the Kronecker delta has been introduced in order to satisfy the choice of β_0 expressed by Eq. (4).

Still with support on the segment $[-1, 1]$ of the real line but with a different functional form, we have the family of measures

$$\mathrm{d}\tau(\xi) = \begin{cases} (1-\xi^2)^{\pm 1/2}\mathrm{d}\xi, & \xi \in [-1, 1], \\ 0, & \text{otherwise}, \end{cases} \tag{14}$$

which is associated with the Chebyshev polynomials of the first kind $\{T_k(\xi)\}$ when the exponent in Eq. (14) is negative, and with the Chebyshev polynomials of the second kind $\{U_k(\xi)\}$ when that exponent is positive. The corresponding sets of monic orthogonal polynomials can be expressed respectively as

$$\Pi_k(\xi) = 2^{-\max(k-1,0)}T_k(\xi), \qquad k \geq 0, \tag{15}$$

for which case the recurrence coefficients are $\alpha_k = 0$ and $\beta_k = \pi\delta_{0,k} + (1-\delta_{0,k})(1+\delta_{1,k})/4$, and

$$\Pi_k(\xi) = 2^{-k}U_k(\xi), \qquad k \geq 0, \tag{16}$$

for which case the recurrence coefficients are $\alpha_k = 0$ and $\beta_k = (\pi/2)\delta_{0,k} + (1-\delta_{0,k})/4$.

For our last example of classical orthogonal polynomials, we consider the measure

$$\mathrm{d}\tau(\xi) = \begin{cases} e^{-\xi}\mathrm{d}\xi, & \xi \geq 0, \\ 0, & \text{otherwise}, \end{cases} \tag{17}$$

which is associated with the Laguerre polynomials $\{L_k(\xi)\}$. The corresponding set of monic orthogonal polynomials is given by

$$\Pi_k(\xi) = (-1)^k k! L_k(\xi), \qquad k \geq 0, \tag{18}$$

and the recurrence coefficients by $\alpha_k = 2k+1$ and $\beta_k = \delta_{0,k} + k^2$.

Finally, we conclude this series of examples with a system of nonclassical orthogonal polynomials that has applications in theoretical chemistry (Wheeler, 1984; Gautschi, 1985). The measure of interest in this case has the peculiarity of having a support that consists of two disjoint intervals, i.e.

$$\mathrm{d}\tau(\xi) = \begin{cases} \pi^{-1}\left|\xi - \frac{1}{2}\right| \left[\xi(1-\xi)(\frac{1}{3}-\xi)(\frac{2}{3}-\xi)\right]^{-1/2}\mathrm{d}\xi, & \xi \in \left[0,\frac{1}{3}\right] \cup \left[\frac{2}{3},1\right], \\ 0, & \text{otherwise}. \end{cases} \tag{19}$$

It turns out that the modified Chebyshev algorithm described next can be used to construct the system of orthogonal polynomials associated with this measure in an accurate way (Wheeler, 1984). In addition, it has been shown (Gautschi, 1984) that the corresponding recurrence coefficients $\{\alpha_k\}$ and $\{\beta_k\}$ can be expressed in closed form, something unusual for nonclassical orthogonal polynomials.

2.3. The Modified Chebyshev Algorithm

Given the system of polynomials $\{\mathcal{P}_k(\xi)\}$ and assuming that the integral in Eq. (9) is computable for $k = 0, 1, \ldots, 2n-1$, we define the vector of modified moments

$$\mathbf{m} = [m_0, m_1, \ldots, m_{2n-1}]^T \tag{20}$$

and note that the modified Chebyshev algorithm is essentially a procedure for implementing the map (Gautschi, 1985)

$$K_n : \Re^{2n} \to \Re^{2n} \qquad \mathbf{m} \to \boldsymbol{\rho}, \tag{21}$$

where $\boldsymbol{\rho}$ is the vector of recurrence coefficients defined by Eq. (7). We also note that if we take $a_k = b_k = 0$ in Eq. (10), the map K_n reduces to the map M_n based on ordinary moments, which becomes exponentially ill-conditioned as n increases, as discussed in Subsection 2.1.

The idea of using modified moments of orthogonal polynomials to avoid the numerical instability of the classical Chebyshev algorithm was introduced by Sack and Donovan (1972). A particularly simple form of the algorithm is due to Wheeler (1974) and has been extensively studied by Gautschi (1978, 1982a, 1985, 1990). The equations that define the modified Chebyshev algorithm in the form proposed by Wheeler are summarized below; for a derivation of these equations see Gautschi (1978, 1990). We first note that the algorithm is based on the *mixed* moments

$$\sigma_{k,l} = \int_{\Re} \Pi_k(\xi)\mathcal{P}_l(\xi)\mathrm{d}\tau(\xi), \tag{22}$$

where $\{\Pi_k(\xi)\}$ are the polynomials that we wish to generate and $\{\mathcal{P}_l(\xi)\}$ are the polynomials introduced in Subsection 2.1, usually referred to as *auxiliary* polynomials. By orthogonality, we have $\sigma_{k,l} = 0$ for $k > l$. The initialization phase of the algorithm is given by

$$\sigma_{-1,l} = 0, \qquad l = 1, 2, \ldots, 2n-2, \tag{23a}$$

$$\sigma_{0,l} = m_l, \qquad l = 0, 1, \ldots, 2n-1, \tag{23b}$$

$$\alpha_0 = a_0 + \frac{m_1}{m_0} \tag{23c}$$

and

$$\beta_0 = m_0, \tag{23d}$$

and the calculation is completed by using the following formulas cyclically, for $k = 1, 2, \ldots, n-1$:

$$\sigma_{k,l} = \sigma_{k-1,l+1} - (\alpha_{k-1} - a_l)\sigma_{k-1,l} - \beta_{k-1}\sigma_{k-2,l} + b_l\sigma_{k-1,l-1}, \qquad l = k, k+1, \ldots, 2n-k-1, \tag{24a}$$

$$\alpha_k = a_k + \frac{\sigma_{k,k+1}}{\sigma_{k,k}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}} \tag{24b}$$

and

$$\beta_k = \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}}. \tag{24c}$$

Gautschi (1982a, 1985, 1990) has performed a sensitivity analysis of the map K_n. His main conclusion was that the sensitivity of this map depends on the magnitude of a polynomial [expressed in terms of the elementary Hermite interpolation polynomials associated with the Gauss nodes generated by $\mathrm{d}\tau(\xi)$] on the support of $\mathrm{d}s(\xi)$, the measure associated with the set of auxiliary orthogonal polynomials. The study of some typical examples (Gautschi, 1982a; 1985; 1990) has led to the general recommendation that the auxiliary orthogonal polynomials should be chosen so that the support of their measure $\mathrm{d}s(\xi)$ coincides with the support of the measure $\mathrm{d}\tau(\xi)$ associated with the polynomials that are being generated.

Finally, we should mention that the main difficulty with the modified Chebyshev algorithm is usually the accurate computation of the modified moments defined by Eq. (9), which are needed in the initialization phase of the algorithm. Sometimes, these moments can be expressed in closed form; in the event that a closed form expression for the moments cannot be found, one should try developing recurrence formulas or using discretization procedures (Gautschi, 1982a; 1985).

2.4. The Discretized Stieltjes Procedure

The so-called Stieltjes procedure is based on the observation that it is possible to obtain explicit formulas for the recurrence coefficients α_k and β_k in Eq. (3) if we multiply that equation by $\Pi_l(\xi)\mathrm{d}\tau(\xi)$ and integrate the resulting equations for $l = k$ and $l = k-1$ over the real line (Gautschi, 1982a; 1985; 1990). Defining the inner product

$$(X, Y) = \int_{\Re} X(\xi)Y(\xi)\mathrm{d}\tau(\xi), \tag{25}$$

we obtain, respectively,

$$\alpha_k = \frac{(\xi\Pi_k, \Pi_k)}{(\Pi_k, \Pi_k)}, \qquad k = 0, 1, \dots, n-1, \tag{26a}$$

and

$$\beta_k = \frac{(\Pi_k, \Pi_k)}{(\Pi_{k-1}, \Pi_{k-1})}, \qquad k = 1, 2, \dots, n-1. \tag{26b}$$

Given a way of computing these inner products accurately, we could, in principle, use Eqs. (26) in alternation with Eq. (3) to find the required recurrence coefficients. The procedure would be the following. First of all, α_0 could be computed from Eq. (26a) with $k = 0$, while $\beta_0 = m_0 = (\Pi_0, \Pi_0)$ by convention. We could then use Eq. (3) with $k = 0$ to generate $\Pi_1(\xi)$. Having generated $\Pi_1(\xi)$, we could use Eqs. (26) with $k = 1$ to compute α_1 and β_1, which could in turn be used in Eq. (3) with $k = 1$ to generate $\Pi_2(\xi)$. Proceeding further for increasing values of k, we would be able to compute all of the required α_k and β_k.

At first glance, one could have the impression that analytical integration, easily applicable if the Π-polynomials are expressed in terms of powers of ξ, would be a good way of evaluating the inner products in Eqs. (26). Unfortunately, this idea is useless because it is equivalent to implementing the map M_n based on the ordinary moments, which is, as discussed in Subsection 2.1, extremely ill-conditioned for large n. In addition, the obvious choice of using the Gaussian quadrature associated with $d\tau(\xi)$ to approximate the integrals that define the inner products is simply not available, because the coefficients $\{\alpha_k\}$ and $\{\beta_k\}$ would have to be known in advance in order to generate such a quadrature. Nevertheless, the approximation of inner products by discrete sums is the central idea of the *discretized* Stieltjes procedure proposed by Gautschi (1968a) and discussed next.

The case of a discrete measure, i.e. a measure that is zero everywhere except for a set of discrete points on the real line, is straightforward, since the integrals that define the inner products in Eqs. (26) reduce to sums. The case of a measure of the form $d\tau(\xi) = \Psi(\xi)d\xi$, where $\Psi(\xi) \geq 0$ for $\xi \in [a, b]$ and $\Psi(\xi) = 0$, otherwise, can be handled as follows (Gautschi, 1968a; 1982a). First we note that the interval $[-1, 1]$ can be mapped onto $[a, b]$ by means of the linear transformation $\xi = \frac{1}{2}(b-a)\eta + \frac{1}{2}(b+a)$. A quadrature rule of the type

$$\int_{-1}^{1} f(\eta)d\eta = \sum_{i=1}^{N} \omega_i f(\eta_i), \tag{27}$$

where $\{\eta_i\}$ and $\{\omega_i\}$ denote respectively the nodes and weights and $N > n$ the order of the quadrature, is then mapped onto $[a, b]$ and used to evaluate the integrals in Eqs. (26). Denoting the transformed nodes as $\xi_i = \frac{1}{2}(b-a)\eta_i + \frac{1}{2}(b+a)$, we can express β_0 as

$$\beta_0 = \frac{1}{2}(b-a)\sum_{i=1}^{N} \omega_i \Psi(\xi_i) \tag{28}$$

and Eqs. (26) as

$$\alpha_k = \frac{\sum_{i=1}^{N} \omega_i \Psi(\xi_i)\xi_i \Pi_k^2(\xi_i)}{\sum_{i=1}^{N} \omega_i \Psi(\xi_i)\Pi_k^2(\xi_i)}, \qquad k = 0, 1, \dots, n-1, \tag{29a}$$

and

$$\beta_k = \frac{\sum_{i=1}^{N} \omega_i \Psi(\xi_i) \Pi_k^2(\xi_i)}{\sum_{i=1}^{N} \omega_i \Psi(\xi_i) \Pi_{k-1}^2(\xi_i)}, \qquad k = 1, 2, \ldots, n-1. \tag{29b}$$

As a quadrature rule recommended for general applications, Gautschi (1968a, 1982a, 1985, 1990) suggests the use of Fejér's rule (Fejér, 1933; Davis and Rabinowitz, 1984). This is the interpolatory rule associated with the Chebyshev nodes $\eta_i = \cos[(2i-1)\pi/(2N)]$, $i = 1, 2 \ldots, N$, and has the advantage, since the corresponding weights ω_i are also expressible in closed form, of requiring less computer time to be generated than, for example, a Gauss-Legendre quadrature of the same order. On the other hand, Fejér's rule of order N integrates exactly polynomials of order up to $N-1$, while the Gauss-Legendre rule of order N does the same up to order $2N-1$.

The cases of semi-infinite and infinite intervals of support can be handled in a similar way by mapping the interval $[-1, 1]$ onto $[0, \infty)$ and $(-\infty, \infty)$ by means of the transformations $\xi = (1+\eta)/(1-\eta)$ and $\xi = \eta/(1-\eta^2)$, $\eta \in [-1, 1]$, respectively (Gautschi, 1968a). In addition, other cases can be devised (for example, a measure with support defined by a number of disjoint intervals) where a composite rule is required (Gautschi, 1982a; 1990). There are also some special cases (Gautschi 1982a; 1985) for which quadrature rules other than Fejér's are known to perform better.

2.5. The Linear-Factor Modification Algorithm

Frequently, the following problem is encountered in the constructive theory of orthogonal polynomials: given a nonnegative measure $d\tau(\xi)$, supported on $[a, b]$ and expressed as a polynomial $p_j(\xi)$ of degree j times another nonnegative measure $ds(\xi)$ supported on the same interval, construct the set of *modified* orthogonal polynomials $\{\Pi_k(\xi)\}$ associated with $d\tau(\xi)$, assuming that the set of *original* orthogonal polynomials $\{\mathcal{P}_k(\xi)\}$ associated with $ds(\xi)$ is available.

An explicit solution to this problem is given by the classical formula of Christoffel (Christoffel, 1858; Szegö, 1939). However, being expressed in determinantal form, Christoffel's formula is not convenient for computational purposes. A more efficient procedure is to compute the recurrence coefficients $\{\alpha_k\}$ and $\{\beta_k\}$ for the modified polynomials directly from those for the original polynomials by using an algorithmic implementation of Christoffel's formula known as the linear-factor modification algorithm (Galant, 1971; Gautschi, 1982b; 1990).

Since a polynomial can always be factored as a product of linear factors, we note that it is sufficient to consider the case where the polynomial $p_j(\xi)$ that multiplies the measure $ds(\xi)$ is of degree $j = 1$. The most general case can then be treated as a sequence of linear cases. For $j = 1$, we can write Christoffel's formula as

$$\Pi_k(\xi) p_1(\xi) = c_k \begin{vmatrix} \mathcal{P}_k(\xi) & \mathcal{P}_{k+1}(\xi) \\ \mathcal{P}_k(r) & \mathcal{P}_{k+1}(r) \end{vmatrix} \tag{30}$$

or, more explicitly, as

$$\Pi_k(\xi)(\xi - r) = c_k[\mathcal{P}_k(\xi)\mathcal{P}_{k+1}(r) - \mathcal{P}_{k+1}(\xi)\mathcal{P}_k(r)], \tag{31}$$

where $r \leq a$ denotes the root of the polynomial $p_1(\xi)$ (the modification needed to handle the case $r \geq b$ will be presented at the end of this subsection) and $c_k = -1/\mathcal{P}_k(r)$ is a normalization constant, chosen so that the coefficient of the highest power in $\Pi_k(\xi)$ be unity. In addition, the original polynomials

$\{\mathcal{P}_k(\xi)\}$ satisfy a three-term recurrence relation of the form of Eq. (10) with known coefficients $\{a_k\}$ and $\{b_k\}$.

A detailed derivation of the linear-factor modification algorithm was presented by Gautschi (1982b), following the arguments of Stiefel (1958). Recently, an alternative derivation of the algorithm has also been made available (Chalhoub and Garcia, 1998). The final result is that the desired recurrence coefficients are computed in terms of those for the original polynomials by performing the following calculations, for $k = 0, 1, \dots, n-1$:

$$\alpha_k = q_k + e_k + r, \tag{32a}$$

and

$$\beta_k = \begin{cases} q_0 b_0, & k = 0, \\ q_k e_{k-1}, & k > 0, \end{cases} \tag{32b}$$

where $q_k = a_k - e_{k-1} - r$ and $e_k = b_{k+1}/q_k$, with $e_{-1} = 0$. Note that these formulas require the knowledge of the coefficients $\{a_k\}$ for $k = 0, 1, \dots, n-1$, while the coefficients $\{b_k\}$ are required for $k = 0, 1, \dots, n$. For the case where the root of the polynomial $p_1(\xi)$ is located to the right of the support interval $[a, b]$, i.e. $p_1(\xi) = r - \xi$, with $r \geq b$, it can be shown that the above formulas are still valid, except that $|q_0|$ replaces q_0 in Eq. (32b). So far, the experience accumulated with the use of the linear-factor modification algorithm suggests that it is numerically stable (Gautschi, 1990).

2.6. The Linear-Divisor Modification Algorithm

The linear-divisor modification algorithm is a procedure that can be used to compute the recurrence coefficients $\{\alpha_k\}$ and $\{\beta_k\}$ for the orthogonal polynomials associated with the nonnegative measure $\mathrm{d}\tau(\xi) = \mathrm{d}s(\xi)/(\xi - r)$, given the recurrence coefficients $\{a_k\}$ and $\{b_k\}$ for the orthogonal polynomials associated with the nonnegative measure $\mathrm{d}s(\xi)$ supported on the finite interval $[a, b]$. The equations that define the algorithm can be readily obtained by considering the *generalized* Christoffel theorem (Uvarov, 1959; 1969) or by inverting the linear-factor modification algorithm discussed in Subsection 2.5 (Gautschi, 1982b; 1990). Defining

$$H(r) = \frac{1}{b_0} \int_a^b \frac{\mathrm{d}s(\xi)}{\xi - r}, \tag{33}$$

we can write the resulting equations as

$$\alpha_0 = \frac{1}{H(r)} + r \tag{34a}$$

and

$$\beta_0 = b_0 H(r), \tag{34b}$$

and, for $k = 1, 2, \dots, n-1$,

$$e_{k-1} = a_{k-1} - q_{k-1} - r, \tag{35a}$$

$$q_k = \frac{b_k}{e_{k-1}}, \tag{35b}$$

$$\alpha_k = q_k + e_{k-1} + r \tag{35c}$$

and

$$\beta_k = q_{k-1}e_{k-1}, \tag{35d}$$

with $q_0 = 1/H(r)$. A slight variant of this algorithm can be employed to handle the case where $\xi - r$ is changed to $|\xi - r|$ in the definition of the measure $d\tau(\xi)$: the above formulas are still valid, except that $H(r)$ must be replaced by $|H(r)|$ in Eq. (34b).

Concerning the stability of the linear-divisor modification algorithm, Gautschi (1982b, 1990) pointed out that it becomes progressively worse as r moves away from the vicinity of the support interval $[a, b]$. Thus, the most important application of this algorithm is undoubtedly in the generation of Gaussian quadrature rules for integration of functions with poles located near the interval of integration (Gautschi, 1990).

2.7. Other Algorithms

In addition to the algorithms discussed in previous subsections, there are a few other algorithms for constructing orthogonal polynomials that have been reported in the literature. Among these, there is an important generalization due to Gautschi (1982b), who showed that the modification of a measure by a rational function $u_l(\xi)/v_m(\xi)$, where $u_l(\xi)$ and $v_m(\xi)$ are, respectively, polynomials of degree l and m, can be achieved in the real domain by a sequence of modifications by linear or quadratic factors and divisors. Explicit forms of the algorithms of modification by quadratic factors and divisors were developed (Gautschi, 1982b; 1990) by using the corresponding linear algorithms twice in sequence. Both of these algorithms share the stability characteristics of their linear counterparts.

3. GENERAL APPLICATIONS

Having discussed their underlying constructive theory and related algorithms, we now turn our attention to general applications of orthogonal polynomials. Generation of Gaussian quadrature rules is the application that appears most frequently in the literature (and that is also the most relevant here), therefore we discuss this topic first. Other types of applications are discussed subsequently. In our presentation, we assume that the recurrence coefficients $\{\alpha_k\}$ and $\{\beta_k\}$ for the set of orthogonal polynomials $\{\Pi_k(\xi)\}$ associated with the measure $d\tau(\xi)$ have been computed by any of the methods discussed in the preceding section.

3.1. Generation of Gaussian Quadrature Rules

A particularly efficient and accurate method for computing the nodes $\{\xi_i\}$ and weights $\{\nu_i\}$ of the Gaussian quadrature rule of order n associated with $d\tau(\xi)$ was introduced by Golub and Welsch (1969).

In short, since the Gaussian nodes ξ_i, $i = 1, 2, \ldots, n$, are the zeros of the polynomial $\{\Pi_n(\xi)\}$ associated with the measure $d\tau(\xi)$, it can be concluded (Golub and Welsch, 1969; Gautschi, 1985) that they are also the eigenvalues of the Jacobi matrix

$$\mathbf{J} = \begin{pmatrix} \alpha_0 & \sqrt{\beta_1} & & & & \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & \\ & \sqrt{\beta_2} & \alpha_2 & \sqrt{\beta_3} & & \\ & & \ddots & \ddots & \ddots & \\ & & & \sqrt{\beta_{n-2}} & \alpha_{n-2} & \sqrt{\beta_{n-1}} \\ & & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{pmatrix}. \tag{36}$$

Moreover, as a consequence of the Christoffel-Darboux identity (Golub and Welsch, 1969), the weights $\{\nu_i\}$ are given by

$$\nu_i = m_0 u_{i,1}^2, \qquad i = 1, 2, \ldots, n, \tag{37}$$

where m_0 is the first moment of $\mathrm{d}\tau(\xi)$, as given by Eq. (9) with $k = 0$, and $u_{i,1}$ is the first component of $\mathbf{u}_i$, the *normalized* eigenvector that satisfies

$$\mathbf{J}\mathbf{u}_i = \xi_i \mathbf{u}_i, \qquad \mathbf{u}_i^T \mathbf{u}_i = 1. \tag{38}$$

Golub and Welsch (1969) proposed the use of the QR algorithm (Francis, 1961; 1962), modified so that only the first components of the eigenvectors are computed, for solving the relevant symmetric tridiagonal eigensystem. The main advantage of using the QR algorithm for computing the eigenvalues and eigenvectors of a band symmetric matrix is that the bandwidth is preserved during the transformation process.

A procedure based on a similar modification of the implicit QL algorithm (Dubrulle *et al.*, 1968), as implemented, for example, in the *Imtql2* routine of the EISPACK package (Smith *et al.*, 1976), was suggested by Gautschi (1979). The advantage of using the implicit QL algorithm to find the eigenvalues and eigenvectors of a symmetric tridiagonal matrix is that it has improved convergence characteristics when compared to the QR algorithm.

3.2. Computation of Functions of the Second Kind

It is well known that the set of orthogonal polynomials $\{\Pi_k(\xi)\}$ can be accurately computed for any desired value of the argument ξ by using Eq. (3) in the forward direction for $k = 0, 1, \ldots$. Similarly, any derivative of $\Pi_k(\xi)$ can be accurately computed by differentiating Eq. (3) as many times as required and using the resulting recurrence relation in the forward direction (note that the recurrence relation for a derivative of order m involves also the derivative of order $m - 1$).

However, in regard to the functions of the second kind

$$\rho_k(z) = \int_{\Re} \Pi_k(\xi) \frac{\mathrm{d}\tau(\xi)}{z - \xi}, \tag{39}$$

defined for $k \geq 0$ and for any complex z not in the support of $\mathrm{d}\tau(\xi)$, the situation is a little different. It can be shown that these functions satisfy the same recurrence relation as the polynomials $\{\Pi_k(\xi)\}$, that is

$$\rho_{k+1}(\xi) = (\xi - \alpha_k)\rho_k(\xi) - \beta_k \rho_{k-1}(\xi), \qquad k = 0, 1, \ldots, \tag{40}$$

but with initial values $\rho_0(z) = \int_{\Re} \mathrm{d}\tau(\xi)/(z-\xi)$ and $\rho_{-1}(z) = 1$, if β_0 is defined as in Eq. (4). In addition, the functions $\{\rho_k(z)\}$ constitute a *minimal solution* (Gautschi, 1967; 1981) of the recurrence relation, in the sense that

$$\lim_{k \to \infty} \frac{\rho_k(z)}{\Pi_k(z)} = 0, \tag{41}$$

provided that the measure $\mathrm{d}\tau(\xi)$ gives rise to a *determined* moment problem (Gautschi, 1981; 1990). Under this condition, the functions $\{\rho_k(z)\}$ can be computed accurately by using Eq. (40) in the *backward* direction, as long as the two required starting values (or at least their ratio) are available (Gautschi, 1967).

3.3. Evaluation of Orthogonal Expansions

When a function $f(\xi)$ is expanded in a set of orthogonal polynomials $\{\Pi_k(\xi)\}$ and the resulting expansion is truncated after the first $n+1$ terms, one is in fact approximating $f(\xi)$ by the partial sum

$$s_n(\xi) = \sum_{k=0}^{n} c_k \Pi_k(\xi). \tag{42}$$

By orthogonality, it is clear that the expansion coefficients $\{c_k\}$ in Eq. (42) can be expressed for $k = 0, 1, \ldots, n$ as

$$c_k = \frac{1}{N_k} \int_{\Re} f(\xi) \Pi_k(\xi) \mathrm{d}\tau(\xi), \tag{43}$$

where N_k is the normalization constant given by Eq. (5). An efficient way of computing partial sums of the form of Eq. (42) is Clenshaw's algorithm (Clenshaw, 1955; Gautschi, 1990):

$$y_{n+1}(\xi) = 0, \tag{44a}$$

$$y_n(\xi) = c_n, \tag{44b}$$

$$y_k(\xi) = (\xi - \alpha_k) y_{k+1}(\xi) - \beta_{k+1} y_{k+2}(\xi) + c_k, \quad k = n-1, n-2, \ldots, 0, \tag{44c}$$

and

$$s_n(\xi) = y_0(\xi). \tag{44d}$$

We note that there are situations for which an alternative form of Clenshaw's algorithm based on forward recurrence should be employed in order to avoid loss of accuracy in the calculation (Press *et al.*, 1986).

3.4. Padé Approximation

Padé formulas are widely used to approximate functions with poles (Baker, 1975). The Padé approximant $f[m,n](z)$ to $f(z)$ is a rational function with a polynomial of degree m in the numerator and a polynomial of degree n in the denominator, constructed so that its power series expansion agrees to as many terms as possible with the power series expansion of $f(z)$, viz.

$$f(z) = \mu_0 + \mu_1 z + \mu_2 z^2 + \cdots. \tag{45}$$

In particular, it is the case for which the coefficients μ_k in Eq. (45) correspond to the ordinary moments of a measure $\mathrm{d}\tau(\xi)$ [see Eq. (1)], that is of interest to us here. In this situation, the theory of Padé approximation becomes closely related to the theory of orthogonal polynomials and Gaussian integration (Gautschi, 1990). For example, when $m = n - 1$ the Padé approximant is in this case (Gautschi, 1990)

$$f[n-1,n](z) = \sum_{i=1}^{n} \frac{\nu_i}{1 - \xi_i z}, \tag{46}$$

where $\{\xi_i\}$ and $\{\nu_i\}$ are respectively the nodes and weights of the Gaussian quadrature of order n associated with the measure $\mathrm{d}\tau(\xi)$.

3.5. Other General Applications

For brevity, we conclude this section by just enumerating other general-purpose applications of orthogonal polynomials that have been described in the literature. Thus, our list of additional applications consists of: iterative methods in linear algebra (Stiefel, 1958); approximation by step functions and splines, summation of series and computation of Cauchy principal value integrals (Gautschi, 1985); and constrained least-squares approximation (Gautschi, 1990).

4. NONCLASSICAL APPLICATIONS IN PARTICLE TRANSPORT THEORY

The phenomenon of particle transport can be modeled mathematically by an integro-differential equation, known in general as the *transport* (or *Boltzmann*) *equation* (Case and Zweifel, 1967). One of the most widely used methods for solving this equation is the discrete-ordinates method (Wick, 1943; Chandrasekhar, 1950; Bell and Glasstone, 1970), which is based on approximating the integral in the transport equation by a quadrature. Therefore, it is not surprising that the majority of the transport-theory applications of nonclassical orthogonal polynomials discussed in this section are concerned with the generation of special quadrature rules for use in the discrete-ordinates method.

In addition, it should be noted here that there is a set of orthogonal polynomials known as the Chandrasekhar polynomials which plays a fundamental role in transport theory, specially when anisotropic scattering is involved (see, for example, İnönü, 1970). These polynomials are shown to be the coefficients in a Legendre polynomial expansion of the eigenfunctions used in the (formally) exact singular-eigenfunction expansion method, also known as Case's method (Case, 1960; Mika, 1961; Case and Zweifel, 1967; McCormick and Kuščer, 1973). They also appear in the context of approximate methods for solving transport problems, e.g. the spherical-harmonics method (Davison, 1950) and the Wick-Chandrasekhar discrete-ordinates method (Wick, 1943; Chandrasekhar, 1950). Strictly speaking, the Chandrasekhar polynomials cannot be considered nonclassical polynomials, since their basic properties can all be derived from the classical Chebyshev theory (Shohat, 1934), as discussed by İnönü (1970). Therefore, these polynomials are not discussed in this work; however, the interested reader can find their recurrence relation, normalization integral, associated measure, quadrature rule and other properties in the work of İnönü (1970) for the azimuthally symmetric case. These properties (with the exception of the quadrature rule) have been generalized for the azimuthally dependent case by McCormick and Veeder (1978). Quite recently, some new identities for the Chandrasekhar polynomials as used in the spherical-harmonics method have been derived by Siewert and McCormick (1997).

In the following subsections, various applications of nonclassical orthogonal polynomials that have been reported in the literature are presented and discussed.

4.1. Evaluation of Mean Intensities and Fluxes in Radiative Transfer

To our knowledge, this is the first application of nonclassical orthogonal polynomials in the field of transport theory. The problem here is to evaluate the integrals (Chandrasekhar, 1950)

$$J(\tau) = \frac{1}{2}\int_0^\infty \mathfrak{J}(t)E_1(|t-\tau|)\mathrm{d}t \tag{47a}$$

and

$$F(\tau) = 2\int_{\tau}^{\infty} \mathfrak{J}(t)E_2(t-\tau)\mathrm{d}t - 2\int_0^{\tau} \mathfrak{J}(t)E_2(\tau - t)\mathrm{d}t, \tag{47b}$$

where $\mathfrak{J}(t)$ is a given function and $E_m(x)$ denotes the mth exponential integral, defined as

$$E_m(x) = \int_1^{\infty} e^{-xt}\frac{\mathrm{d}t}{t^m}, \qquad m \geq 1. \tag{48}$$

Since $E_1(x)$ and the derivative of $E_2(x)$ have logarithmic singularities at $x = 0$, evaluating the integrals in Eqs. (47) with special quadrature rules generated by measures that include these functions in their definitions is clearly better than evaluating these integrals with standard quadrature rules.

Chandrasekhar (1950) used a change of variables to rewrite Eqs. (47) in the forms

$$J(\tau) = \frac{1}{2}\int_0^{\infty} \mathfrak{J}(\tau+\xi)E_1(\xi)\mathrm{d}\xi + \frac{1}{2}\int_0^{\tau} \mathfrak{J}(\tau-\xi)E_1(\xi)\mathrm{d}\xi \tag{49a}$$

and

$$F(\tau) = 2\int_0^{\infty} \mathfrak{J}(\tau+\xi)E_2(\xi)\mathrm{d}\xi - 2\int_0^{\tau} \mathfrak{J}(\tau-\xi)E_2(\xi)\mathrm{d}\xi, \tag{49b}$$

and applied a method based on the solution of a linear system and the determination of the roots of a polynomial to compute and tabulate the nodes and weights of some low-order ($n \leq 3$) Gaussian quadratures associated with the measures $E_m(\xi)\mathrm{d}\xi$, $m = 1$ and 2, on the support intervals $[0,\infty)$ and $[0,\tau]$, for several values of the optical variable τ. However, Chandrasekhar's method of generating the required Gaussian quadrature rules is of limited use, because it is based on the ordinary moments of the associated measures, and, as discussed in Section 2, such methods display an ill-conditioned behavior that grows exponentially with n. This difficulty was overcome by Gautschi (1968a) who proposed the use of the discretized Stieltjes procedure (see Subsection 2.4) to generate the required Gaussian quadrature rules. A 20-point rule for the measure $E_1(\xi)\mathrm{d}\xi$ on $[0,\infty)$ was reported in a subsequent publication (Gautschi, 1968b).

4.2. Chemical Kinetics

The first application of nonclassical orthogonal polynomials in the solution of chemical kinetics problems is due to Shizgal (1981a). A typical problem in this area is that of solving the Boltzmann equation for the reactive system (Shizgal and Karplus, 1971)

$$\mathrm{A} + \mathrm{B} \rightarrow \text{products}, \tag{50}$$

where species B is assumed to be present in large excess and at equilibrium. Then, $\phi(x)$, the perturbation of the distribution function for species A from the usual equilibrium Maxwellian energy distribution $M(x) = 2(x/\pi)^{1/2}e^{-x}$, where $x = mc^2/(2kT)$ denotes the reduced translational energy, is described by the integral equation

$$\int_0^{\infty} K(x',x)M(x')\phi(x')\mathrm{d}x' - Z(x)M(x)\phi(x) = -M(x)\left[R(x) - \int_0^{\infty} M(x')R(x')\mathrm{d}x'\right], \tag{51}$$

where $K(x',x)$ is the Wigner-Wilkins kernel, $Z(x)$ is the elastic collision frequency and $R(x)$ is the reactive collision frequency (Shizgal, 1981a). Moreover, the quantity of interest in this problem,

$$\eta = \frac{\int_0^{\infty} M(x)\phi(x)R(x)\mathrm{d}x}{\int_0^{\infty} M(x)R(x)\mathrm{d}x}, \tag{52}$$

characterizes the departure from equilibrium of species A in an integral sense, and can be readily computed once Eq. (51) is solved for $\phi(x)$.

In order to solve Eq. (51) subject to the auxiliary condition

$$\int_0^{\infty} M(x)\phi(x)\mathrm{d}x = 0, \tag{53}$$

Shizgal (1981a) implemented the discrete-ordinates method. In the course of the implementation, integrals of the form $\int_0^{\infty} e^{-x^2}x^p f(x)\mathrm{d}x$, $p = 0$, 1 and 2, were approximated by the Gaussian quadrature rules associated with the nonclassical measures $e^{-x^2}x^p\mathrm{d}x$, $p = 0$, 1 and 2, supported on $[0,\infty)$. An *ad hoc* algorithm based on Christoffel-Darboux formulas was developed and used by Shizgal (1981a) to compute the recurrence coefficients for the associated orthogonal polynomials. Unfortunately, the algorithm was found to be numerically unstable, and so the calculation had to be implemented in multiple-precision arithmetic to avoid excessive loss of accuracy. Later on, Gautschi (1990) used, for the case $p = 0$, the discretized Stieltjes procedure discussed in Subsection 2.4 to obtain nodes and weights accurate to 12 significant figures for a quadrature of order $n = 40$, using a 81-point Fejér rule in each of the following four subintervals: $[0,3]$, $[3,6]$, $[6,9]$ and $[9,\infty)$.

A comparison of discrete-ordinates results obtained for η using the specially developed Gauss formulas to solve the problem with similar results obtained with the use of the Gauss-Laguerre formula (the obvious classical choice for this problem) showed a faster convergence rate for the former, as the order of the quadrature was increased (Shizgal, 1981a).

To close this subsection, we note that the nonstandard quadrature rule generated by Shizgal (1981a) for $p = 2$ was also applyed in discrete-ordinates solutions of the Boltzmann equations relevant to time-dependent studies of hot atom systems (Shizgal, 1981b) and in (discrete-ordinates) eigenvalue calculations of the Boltzmann collision operator (Shizgal *et al.*, 1981; Shizgal and Blackmore, 1983). In addition, it has been used to solve eigenvalue problems associated with Lorentz-Fokker-Planck equations relevant to the study of electron transport phenomena in gases (Shizgal, 1983; Shizgal and McMahon, 1984; 1985; McMahon and Shizgal, 1985).

4.3. Solution of Fokker-Planck Equations with Nonlinear Coefficients

As discussed by Blackmore and Shizgal (1985), Fokker-Planck equations with nonlinear coefficients are used to model nonequilibrium processes in chemically reactive systems, laser systems and many other applications. These authors considered a Fokker-Planck equation of the form

$$\frac{\partial}{\partial t}P(x,t) = \frac{\partial}{\partial x}\left[A(x)P(x,t)\right] + \frac{\partial^2}{\partial x^2}\left[B(x)P(x,t)\right], \tag{54}$$

where $P(x,t)$ is the probability density function and gives the probability that a macroscopic property of the system being studied will take on a specific value x at time t, and $A(x)$ and $B(x)$ are respectively the (known) drift and diffusion coefficients. This equation can be written more compactly as

$$\frac{\partial}{\partial t}P(x,t) = \tilde{L}P(x,t), \tag{55}$$

where $\tilde{L}$ denotes the Fokker-Planck operator. Using the eigenfunction expansion method and considering the boundary conditions $P(\pm\infty,t) = 0$, Blackmore and Shizgal (1985) wrote the solution to Eq. (55) as

$$P(x,t) = \sum_{m=0}^{\infty} a_m e^{-\lambda_m t} P_m(x), \tag{56}$$

where the eigenvalues $\{\lambda_m\}$ and the eigenfunctions $\{P_m(x)\}$ satisfy, for $m = 0, 1, \ldots,$

$$\tilde{L}P_m(x) = -\lambda_m P_m(x), \tag{57}$$

and the coefficients $\{a_m\}$ are expressed in terms of the initial probability density function $P(x, 0)$ as

$$a_m = \int_{-\infty}^{\infty} P_0^{-1}(x) P_m(x) P(x, 0) \mathrm{d}x. \tag{58}$$

Here, the eigenfunction $P_0(x)$ is the stationary solution of Eq. (55) and is given by

$$P_0(x) = N \exp\left[-\int_0^x \frac{A(x')}{B(x')} \mathrm{d}x' - \ln B(x)\right], \tag{59}$$

where N represents a normalization constant chosen so that $\int_{-\infty}^{\infty} P_0(x)\mathrm{d}x = 1$. Clearly, the corresponding eigenvalue λ_0 is zero.

The *discrete-ordinate method* (Shizgal and Blackmore, 1984), also termed, perhaps more appropriately, *quadrature discretization method* (Shizgal, 1992), was implemented by Blackmore and Shizgal (1985) to find the eigenvalues and eigenfunctions of the Fokker-Planck operator for the case

$$A(x) = gx^3 - ax \tag{60a}$$

and

$$B(x) = \epsilon, \tag{60b}$$

where g, a and ϵ are parameters. The underlying idea of the quadrature discretization method is to represent derivative operators in a discrete space defined by the nodes of a Gaussian quadrature rule. In the present case, a Gaussian rule that was judged to be a good choice for fast convergence of Eq. (56) is the rule associated with a nonstandard measure supported on the entire real line and proportional to $e^{-\gamma x^4/2 + \alpha x^2}\mathrm{d}x$, where γ and α are related to the parameters in Eqs. (60). Since this measure is symmetric with respect to $x = 0$, the recurrence coefficients $\{\alpha_k\}$ for the corresponding orthogonal polynomials all vanish. The recurrence coefficients $\{\beta_k\}$ were computed with a method based on a Christoffel-Darboux formula (Blackmore and Shizgal, 1985). As before (Shizgal, 1981a), the resulting algorithm was found to be unstable in high-order, and consequently a multiple-precision package was required to generate these coefficients accurately.

4.4. Azimuthally Dependent Problems

A class of transport problems that has received increasing attention in recent years is that of azimuthally dependent problems. Besides the more traditional applications in astrophysics (Chandrasekhar, 1950) and nuclear-reactor shielding (Goldstein, 1959; Selph, 1973), such problems have also found important applications in atmospheric radiative transfer (Liou, 1980) and hydrologic optics (Mobley, 1994).

The azimuthally dependent transport equation for a homogeneous plane-parallel medium can be written, in the absence of internal sources, as (Chalhoub and Garcia, 1997)

$$\mu \frac{\partial}{\partial x} \psi(x, \mu, \varphi) + \sigma_t \psi(x, \mu, \varphi) = \sigma_s \int_{-1}^{1} \int_0^{2\pi} p(\cos \Theta) \psi(x, \mu', \varphi') \mathrm{d}\varphi' \mathrm{d}\mu', \tag{61}$$

where $\psi(x, \mu, \varphi)$ is the particle angular flux, $x \in (0, a)$ is the space variable measured in unit length, $\mu \in [-1, 1]$ and $\varphi \in [0, 2\pi]$ are, respectively, the cosine of the polar angle and the azimuthal angle that specify the direction of particle motion, and σ_t and σ_s are the total and scattering macroscopic cross sections, respectively. In addition, $p(\cos\Theta)$ denotes the scattering law, which is usually expressed as a truncated Legendre polynomial expansion in terms of the cosine of the scattering angle Θ, i.e.

$$p(\cos\Theta) = \frac{1}{4\pi}\sum_{l=0}^{L}\beta_l P_l(\cos\Theta), \tag{62}$$

where the coefficients $\{\beta_l\}$ must obey the restrictions $\beta_0 = 1$ and $|\beta_l| < 2l+1$, $l = 1, 2, \dots, L$. Along with Eq. (61), we consider the boundary conditions, for $\mu \in (0,1]$ and $\varphi \in [0,2\pi]$,

$$\psi(0,\mu,\varphi) = \pi\delta(\mu-\mu_0)\delta(\varphi-\varphi_0) \tag{63a}$$

and

$$\psi(a,-\mu,\varphi) = 0. \tag{63b}$$

Here, Eq. (63a) represents a particle beam of intensity π striking uniformly the surface $x = 0$ of the medium with a direction specified by $\mu_0 \in (0,1]$ and $\varphi_0 \in [0,2\pi]$, while Eq. (63b) defines the surface $x = a$ as a free boundary.

We now summarize an improved way of implementing ANISN (Engle, 1973), a widely used one-dimensional code for numerically solving the discrete-ordinates version of the problem posed by Eqs. (61–63). The details of this implementation can be found elsewhere (Chalhoub and Garcia, 1997). Following Chandrasekhar (1950), we begin by decomposing the original problem into uncollided and collided components. We write

$$\psi(x,\mu,\varphi) = \psi_0(x,\mu,\varphi) + \psi_*(x,\mu,\varphi), \tag{64}$$

where the uncollided angular flux $\psi_0(x,\mu,\varphi)$ satisfies a version of Eq. (61) with zero right-hand side and boundary conditions similar to Eqs. (63), and is given, for $x \in [0,a]$, $\mu \in [0,1]$ and $\varphi \in [0,2\pi]$, by

$$\psi_0(x,\mu,\varphi) = \pi\delta(\mu-\mu_0)\delta(\varphi-\varphi_0)e^{-\sigma_t x/\mu} \tag{65a}$$

and

$$\psi_0(x,-\mu,\varphi) = 0. \tag{65b}$$

On the other hand, the collided angular flux $\psi_*(x,\mu,\varphi)$ must satisfy

$$\mu\frac{\partial}{\partial x}\psi_*(x,\mu,\varphi) + \sigma_t\psi_*(x,\mu,\varphi) = \sigma_s\int_{-1}^{1}\int_{0}^{2\pi} p(\cos\Theta)\psi_*(x,\mu',\varphi')\mathrm{d}\varphi'\mathrm{d}\mu' + Q(x,\mu,\varphi), \tag{66}$$

where the first-collision source $Q(x,\mu,\varphi)$ is given by

$$Q(x,\mu,\varphi) = \sigma_s\int_{-1}^{1}\int_{0}^{2\pi} p(\cos\Theta)\psi_0(x,\mu',\varphi')\mathrm{d}\varphi'\mathrm{d}\mu', \tag{67}$$

and the boundary conditions, for $\mu \in (0,1]$ and $\varphi \in [0,2\pi]$,

$$\psi_*(0,\mu,\varphi) = \psi_*(a,-\mu,\varphi) = 0. \tag{68}$$

The azimuthal dependence of the collided problem formulated by Eqs. (66–68) can be handled by considering the *finite* Fourier decomposition (Chandrasekhar, 1950)

$$\psi_*(x,\mu,\varphi) = \frac{1}{2}\sum_{m=0}^{L}(2-\delta_{0,m})\psi_*^m(x,\mu)\cos[m(\varphi-\varphi_0)] \tag{69}$$

and using the addition theorem for the Legendre polynomials (Erdélyi *et al.*, 1953) to express the scattering law as

$$p(\cos\Theta) = \frac{1}{4\pi}\sum_{m=0}^{L}(2-\delta_{0,m})\sum_{l=m}^{L}\beta_l P_l^m(\mu)P_l^m(\mu')\cos[m(\varphi-\varphi')], \tag{70}$$

where $P_l^m(\mu)$ denotes a *normalized* associated Legendre function, defined for $l \geq m$ as

$$P_l^m(\mu) = \left[\frac{(l-m)!}{(l+m)!}\right]^{1/2}(1-\mu^2)^{m/2}\frac{\mathrm{d}^m}{\mathrm{d}\mu^m}P_l(\mu). \tag{71}$$

We find that the Fourier component $\psi_*^m(x,\mu)$ of the collided angular flux must satisfy the transport equation

$$\mu\frac{\partial}{\partial x}\psi_*^m(x,\mu) + \sigma_t\psi_*^m(x,\mu) = \frac{\sigma_s}{2}\sum_{l=m}^{L}\beta_l P_l^m(\mu)\int_{-1}^{1}P_l^m(\mu')\psi_*^m(x,\mu')\mathrm{d}\mu' + Q^m(x,\mu), \tag{72}$$

with

$$Q^m(x,\mu) = \frac{\sigma_s}{2}e^{-\sigma_t x/\mu_0}\sum_{l=m}^{L}\beta_l P_l^m(\mu)P_l^m(\mu_0), \tag{73}$$

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

$$\psi_*^m(0,\mu) = \psi_*^m(a,-\mu) = 0. \tag{74}$$

Thus, once Eqs. (72–74) are solved for the Fourier components $\psi_*^m(x,\mu)$, $m = 0,1,\ldots,L$, Eq. (69) can be used to calculate the collided angular flux for any desired values of x, μ and φ.

The improved way of implementing the ANISN code for computing the desired Fourier components $\psi_*^m(x,\mu)$, $m = 0,1,\ldots,L$, is based on the use of the transformation (Chalhoub and Garcia, 1997)

$$\psi_*^m(x,\mu) = (1-\mu^2)^{m/2}F^m(x,\mu) \tag{75}$$

and the associated Legendre *polynomials*

$$D_l^m(\mu) = \left[\frac{(2m)!!}{(2m-1)!!}\right]^{1/2}\left[\frac{(l-m)!}{(l+m)!}\right]^{1/2}\frac{\mathrm{d}^m}{\mathrm{d}\mu^m}P_l(\mu), \tag{76}$$

which are normalized so that $D_m^m(\mu) = 1$, to reformulate the problem given by Eqs. (72–74) as

$$\mu\frac{\partial}{\partial x}F^m(x,\mu) + \sigma_t F^m(x,\mu) = \frac{\sigma_s^m}{2}\sum_{l=m}^{L}\beta_l D_l^m(\mu)\int_{-1}^{1}(1-\mu'^2)^m D_l^m(\mu')F^m(x,\mu')\mathrm{d}\mu' + S^m(x,\mu), \tag{77}$$

where

$$\sigma_s^m = \left[\frac{(2m-1)!!}{(2m)!!}\right]\sigma_s, \tag{78}$$

$$S^m(x,\mu) = \frac{\sigma_s^m}{2}(1-\mu_0^2)^{m/2}e^{-\sigma_t x/\mu_0}\sum_{l=m}^{L}\beta_l D_l^m(\mu)D_l^m(\mu_0), \tag{79}$$

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

$$F^m(0, \mu) = F^m(a, -\mu) = 0. \tag{80}$$

Now, provided a Gaussian quadrature rule based on the measure $(1 - \mu^2)^m \mathrm{d}\mu$ is used to implement the discrete-ordinates method of solution, the first term in the summation on the right-hand side of Eq. (77) can be readily expressed in the form required by ANISN, i.e. a constant times $\sum \omega_i \Phi(x, \mu_i)$, where $\Phi(x, \mu)$ denotes the particle distribution being computed. This is not the case of a previous ANISN implementation (Hill *et al.*, 1974), where artificial terms for $l = 0, 1, \ldots, m - 1$ had to be included in the summation, in order to satisfy this basic ANISN requirement.

It is well known (Bell and Glasstone, 1970) that a composite quadrature rule designed to approximate the integrals in Eq. (77) independently in each of the semi-intervals $[-1, 0]$ and $[0, 1]$ allows for a better representation of the angular-flux discontinuities at the boundaries of the medium for $|\mu| \to 0$ than a single quadrature rule generated for the interval $[-1, 1]$. For this reason, a composite quadrature rule was used in the improved ANISN implementation of Chalhoub and Garcia (1997). As the half-range rules that make up the composite rule are symmetric, it is clearly sufficient to generate the Gaussian quadrature rule for $[0, 1]$ and obtain the rule for $[-1, 0]$ from symmetry considerations.

The modified Chebyshev and linear-factor modification algorithms discussed in Section 2 were used recursively in m (Chalhoub and Garcia, 1998) to generate the recurrence coefficients for the family of orthogonal polynomials associated with the measure $(1 - \mu^2)^m \mathrm{d}\mu$ on the support interval $[0, 1]$. As expected, both algorithms showed a stable behavior and yielded excellent results, but the latter is considered more adequate for this application because it required $\sim 20\%$ less computer time than the former (Chalhoub and Garcia, 1998).

In conclusion, as discussed in detail by Chalhoub and Garcia (1997), this new ANISN implementation is more accurate and efficient than the implementation of Hill *et al.* (1974). Just to give an idea of the kind of improvement in accuracy that can be obtained, the maximum deviation in the angular flux observed using the ANISN implementation of Hill *et. al.* (1974) to solve the H2O problem proposed by Chalhoub and Garcia (1997) was $\sim 25\%$, while with the new implementation the maximum deviation in the angular flux was only $\sim 5\%$.

4.5. Evaluation of Some Integrals for the F_N Method in Atmospheric Radiative Transfer

Recently, an improved version (Garcia and Siewert, 1998) of the F_N method (Siewert and Benoist, 1979; Garcia, 1985; Garcia *et al.*, 1994) has been developed and used to solve a class of azimuthally dependent problems with strong scattering anisotropy. In that work, the integrals

$$A_\alpha^m(\xi) = \varpi \int_0^1 \mu G^m(-\xi, \mu) P_{m+2\alpha}^m(\mu) \frac{\mathrm{d}\mu}{\xi + \mu} \tag{81}$$

were required for a set of values of ξ that consists of the *positive* discrete spectrum $\{\nu_\beta^m\}$, where $\nu_\beta^m \geq 1$, $\beta = 0, 1, \ldots, \aleph^m - 1$, are the $\aleph^m$ positive zeros of the dispersion function (Garcia and Siewert, 1982; 1989)

$$\Lambda^m(\xi) = 1 - \frac{\varpi\xi}{2} \int_{-1}^1 (1 - \mu^2)^{m/2} G^m(\mu, \mu) \frac{\mathrm{d}\mu}{\xi - \mu}, \tag{82}$$

and a subset of points contained in $[0, 1]$, the nonnegative part of the continuum spectrum. In Eq. (81), the integer α runs from 0 to N, the order of the F_N approximation used to solve the problem, and the

Fourier index m from 0 to L, the order of the scattering anisotropy. Furthermore, in Eqs. (81) and (82), $\varpi \in (0,1]$ is the albedo for single scattering and

$$G^m(\xi,\mu) = \sum_{l=m}^{L} \beta_l g_l^m(\xi) P_l^m(\mu), \tag{83}$$

where $g_l^m(\xi)$ denotes a *normalized* Chandrasekhar polynomial (Garcia and Siewert, 1990).

Considering the definition of the associated Legendre function $P_l^m(\mu)$ expressed by Eq. (71), we can see that the integrand in Eq. (81) is given by a polynomial of degree $L + 2\alpha + 1$ in μ times the factor $1/(\xi+\mu)$. Thus, if we take $d\mu/(\xi+\mu)$ as the measure, it is clear that we can integrate Eq. (81) for $\alpha = 0, 1, \ldots, N$ exactly (except for computer round-off errors) if we use the related Gaussian quadrature of order $[L/2] + N + 1$, where $[x]$ denotes the integer part of x. The fact that the integrals can be computed exactly is an advantage of this rule when compared to the standard Gaussian rule (in this case, the Gauss-Legendre rule shifted to [0,1]). On the other hand, the nonstandard rule is specific for ξ, and thus a different rule must be generated for each required value of ξ in Eq. (81).

In the work of Garcia and Siewert (1998), a modified version of the linear-divisor modification algorithm discussed in Subsection 2.6 was used to compute the recurrence coefficients for the set of orthogonal polynomials associated with the measure $d\mu/(\xi+\mu)$, for all required values of ξ in a problem with scattering anisotropy of order $L = 299$ and for which high-order F_N approximations, say $N = 699$, had to be employed in order to obtain accurate results. The modification introduced in the linear-divisor algorithm consists in combining Eqs. (35a) and (35b) into a single recurrence formula for the quantities $\{e_k\}$ and using the resulting formula in the backward direction. With this modification, it became possible to overcome the characteristic unstable behavior of the original linear-divisor modification algorithm in this problem.

4.6. Neutral Particle Transport in Ducts

Some years ago, Larsen *et al.* (1986) developed an approximate model for treating neutral particle transport in ducts of arbitrary cross-sectional geometry. Since their model makes use of two basis functions to represent the transverse (x, y) and azimuthal (φ) dependences of the particle angular flux, they called it "the $N = 2$ model". This model can be considered (Larsen, 1984) a natural extension of the statistical ($N = 1$) model proposed earlier by Prinja and Pomraning (1984), and is described by the matrix transport equation

$$\mu\frac{\partial}{\partial z}\boldsymbol{\Psi}(z,\mu) + (1-\mu^2)^{1/2}\mathbf{A}\boldsymbol{\Psi}(z,\mu) = \frac{2c}{\pi}(1-\mu^2)^{1/2}\mathbf{B}\int_{-1}^{1}(1-\mu'^2)^{1/2}\boldsymbol{\Psi}(z,\mu')d\mu', \tag{84}$$

for $z \in (0, Z)$ and $\mu \in [-1,1]$, and the boundary conditions

$$\boldsymbol{\Psi}(0,\mu) = \mathbf{F}(\mu) \tag{85a}$$

and

$$\boldsymbol{\Psi}(Z,-\mu) = \mathbf{G}(\mu), \tag{85b}$$

for $\mu > 0$. Here $\boldsymbol{\Psi}(z,\mu)$ is a column vector of two components, the unknown coefficients $\Psi_j(z,\mu)$ for $j = 1$ and 2 in the approximate representation of the angular flux

$$\Psi(x,y,z,\mu,\varphi) = \Psi_1(z,\mu)\alpha_1(x,y,\varphi) + \Psi_2(z,\mu)\alpha_2(x,y,\varphi), \tag{86}$$

where the basis functions $\alpha_j(x,y,\varphi)$, $j = 1$ and 2, are specified in the work of Larsen *et al.* (1986). In addition, c is the scattering probability at the duct wall, $\mathbf{A}$ and $\mathbf{B}$ are 2×2 full matrices that depend on the duct cross-sectional geometry and on the prescription of the basis and weight functions (Larsen *et al.*, 1986), Z is the duct lenght and the vectors $\mathbf{F}(\mu)$ and $\mathbf{G}(\mu)$ are assumed known.

Larsen *et al.* (1986) used a numerical implementation of the discrete-ordinates method to solve the problem formulated by Eqs. (84) and (85) and tabulated, for circular ducts, numerical results for the reflection probability

$$R = \frac{\int_0^1 \mu \Psi_1(0,-\mu)d\mu}{\int_0^1 \mu \Psi_1(0,\mu)d\mu} \tag{87a}$$

and the transmission probability

$$T = \frac{\int_0^1 \mu \Psi_1(Z,\mu)d\mu}{\int_0^1 \mu \Psi_1(0,\mu)d\mu}, \tag{87b}$$

as functions of the duct length Z and the wall scattering probability c. While the discrete-ordinates results of Larsen *et al.* (1986) compared well with Monte Carlo results, for some cases of long ducts with significant wall absorption a large number of discrete ordinates (as high as 640) had to be employed, in order to obtain accurate results for the reflection probabilities.

Recently, Garcia and Ono (1999) developed an improved version of the numerical discrete-ordinates method that allowed a substantial reduction in the number of ordinates required to obtain good results for the problem, especially for the difficult cases of long ducts with significant wall absorption. Their formulation is based on a decomposition of the original problem into uncollided and collided problems. The solution to Eqs. (84) and (85) is expressed as

$$\mathbf{\Psi}(z,\mu) = \mathbf{\Psi}_0(z,\mu) + \mathbf{\Psi}_*(z,\mu), \tag{88}$$

where the uncollided component $\mathbf{\Psi}_0(z,\mu)$ satisfies Eq. (84) with $c = 0$ and Eqs. (85), i.e.

$$\mu\frac{\partial}{\partial z}\mathbf{\Psi}_0(z,\mu) + (1-\mu^2)^{1/2}\mathbf{A}\mathbf{\Psi}_0(z,\mu) = \mathbf{0}, \tag{89}$$

for $z \in (0, Z)$ and $\mu \in [-1, 1]$, and

$$\mathbf{\Psi}_0(0,\mu) = \mathbf{F}(\mu) \tag{90a}$$

and

$$\mathbf{\Psi}_0(Z,-\mu) = \mathbf{G}(\mu), \tag{90b}$$

for $\mu > 0$, and the collided component $\mathbf{\Psi}_*(z,\mu)$ satisfies

$$\mu\frac{\partial}{\partial z}\mathbf{\Psi}_*(z,\mu) + (1-\mu^2)^{1/2}\mathbf{A}\mathbf{\Psi}_*(z,\mu) = \frac{2c}{\pi}(1-\mu^2)^{1/2}\mathbf{B}\int_{-1}^{1}(1-\mu'^2)^{1/2}\mathbf{\Psi}_*(z,\mu')d\mu' + \mathbf{Q}(z,\mu), \tag{91}$$

for $z \in (0, Z)$ and $\mu \in [-1, 1]$, and the boundary conditions

$$\mathbf{\Psi}_*(0,\mu) = \mathbf{0} \tag{92a}$$

and

$$\mathbf{\Psi}_*(Z,-\mu) = \mathbf{0}, \tag{92b}$$

for $\mu > 0$. The first-collision source $\mathbf{Q}(z,\mu)$ in Eq. (91) is given by

$$\mathbf{Q}(z,\mu) = \frac{2c}{\pi}(1-\mu^2)^{1/2}\mathbf{B}\int_{-1}^{1}(1-\mu'^2)^{1/2}\mathbf{\Psi}_0(z,\mu')d\mu' \tag{93}$$

and becomes explicitly known once the uncollided problem is solved.

In regard to the uncollided problem, a diagonalization procedure was used by Garcia and Ono (1999) to reduce this problem to a decoupled "two-group" problem for which a solution can be readily found. The resulting uncollided solution can be written as (Garcia and Ono, 1999)

$$\boldsymbol{\Psi}_0(z,\mu) = \left[\mathbf{U}_{12}e^{-\lambda_1(1-\mu^2)^{1/2}z/\mu} + \mathbf{U}_{21}e^{-\lambda_2(1-\mu^2)^{1/2}z/\mu}\right]\mathbf{F}(\mu) \tag{94a}$$

and

$$\boldsymbol{\Psi}_0(z,-\mu) = \left[\mathbf{U}_{12}e^{-\lambda_1(1-\mu^2)^{1/2}(Z-z)/\mu} + \mathbf{U}_{21}e^{-\lambda_2(1-\mu^2)^{1/2}(Z-z)/\mu}\right]\mathbf{G}(\mu), \tag{94b}$$

for $z \in [0, Z]$ and $\mu > 0$, where λ_1 and λ_2 are the (assumed distinct) eigenvalues of $\mathbf{A}$ and

$$\mathbf{U}_{ij} = \frac{1}{\lambda_i - \lambda_j}\begin{pmatrix} \lambda_i - a_{22} & -(\lambda_i - a_{22})(\lambda_j - a_{22})/a_{21} \\ a_{21} & -(\lambda_j - a_{22}) \end{pmatrix}, \tag{95}$$

with a_{ij} denoting the (i, j) element of $\mathbf{A}$. We note that, to avoid the need of using complex arithmetic in the calculation, Eqs. (94) were reformulated in terms of real quantities for the case where the eigenvalues of $\mathbf{A}$ appear as a complex conjugate pair, and that the degenerate case $\lambda_1 = \lambda_2$ was also treated explicitly (Garcia and Ono, 1999).

With the uncollided solution available, a numerical version of the discrete-ordinates method was implemented for solving the collided problem defined by Eqs. (91–93). Using the same Gaussian quadrature based on the Chebyshev polynomials of the second kind that was used by Larsen *et al.* (1986) to approximate the integral term of the transport equation, Garcia and Ono (1999) were able to generate accurate numerical results for the reflection (R) and transmission (T) probabilities with a reduced number of ordinates (in some cases, a reduction of almost an order of magnitude). While such improvement is due to the uncollided/collided decomposition introduced, a further reduction (typically a factor of 1/2) in the number of ordinates necessary to achieve a given level of accuracy in the results for R and T was attained (Garcia and Ono, 1999) by using a composite Gaussian quadrature consisting of two separate quadratures for the intervals $[-1, 0]$ and $[0, 1]$. As the composite quadrature rule is symmetric in this case, the rule for $[-1, 0]$ can be deduced from the rule for $[0, 1]$, and thus it was necessary to generate only the (nonstandard) rule related to the measure $(1 - \mu^2)^{1/2}d\mu$ with support on $[0, 1]$. The modified Chebyshev algorithm discussed in Subsection 2.3 was successfully implemented by Garcia and Ono (1999) to compute the recurrence coefficients for the orthogonal polynomials associated with this measure. Once these coefficients were available, the method discussed in Subsection 3.1 was used to generate the required Gaussian rule accurately.

5. CONCLUDING REMARKS

The high diversity of subjects in the field of transport theory to which nonclassical orthogonal polynomials can be applied is apparent from Section 4 of this paper. Since in our opinion the spectrum of these subjects can still be widened, we hope that this review can be of value to researchers involved in the development and/or improvement of solution methods for transport problems.

Based on our own experience on the subject, we would like to conclude this work with some comments concerning the selection of what could be called the "best" constructive algorithm for a given application. First of all, if the related measure differs only by a linear factor (divisor) or a sequence of such factors (divisors) from another measure for which the associated set of orthogonal polynomials has recurrence coefficients which are explicitly known (e.g. a classical measure) or can be easily computed, then the linear-factor (linear-divisor) modification algorithm discussed in Subsection 2.5 (Subsection 2.6) or the generalized modification algorithm mentioned in Subsection 2.7 should be considered. In case that the given measure cannot be related in such a simple way to a convenient measure, but a set of auxiliary polynomials that follows the general recommendation stated in Subsection 2.3 can be found, the modified Chebyshev algorithm is the natural choice. Finally, if the application is such that none of these algorithms seems appropriate, one should consider using the discretized Stieltjes procedure discussed in Subsection 2.4.

Acknowledgements—The author wishes to acknowledge the financial support received from the Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP) to attend the XI ENFIR meeting. This work was supported in part by the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq).

REFERENCES

Baker, Jr. G. A. (1975) *Essentials of Padé Approximants*, Academic Press, New York.

Bell G. I. and Glasstone S. (1970) *Nuclear Reactor Theory*, Van Nostrand Reinhold, New York.

Blackmore R. and Shizgal B. (1985) Discrete-Ordinate Method of Solution of Fokker-Planck Equations with Nonlinear Coefficients. *Phys. Rev. A* **31**, 1855.

Case K. M. (1960) Elementary Solutions of the Transport Equation and Their Applications. *Ann. Phys.* **9**, 1.

Case K. M. and Zweifel P. F. (1967) *Linear Transport Theory*, Addison-Wesley, Reading, Mass.

Chalhoub E. S. and Garcia R. D. M. (1997) On the Solution of Azimuthally Dependent Transport Problems with the ANISN Code. *Ann. Nucl. Energy* **24**, 1069.

Chalhoub E. S. and Garcia R. D. M. (1998) A New Quadrature Scheme for Solving Azimuthally Dependent Transport Problems. *Transp. Theory Stat. Phys.* **27**, 607.

Chandrasekhar S. (1950) *Radiative Transfer*, Oxford University Press, London.

Chebyshev P. L. (1859) Sur l'Interpolation par la Méthode des Moindres Carrés. *Mém. Acad. Impér. Sci. St. Pétersbourg (7)* **1**, 1.

Chihara T. S. (1978) *An Introduction to Orthogonal Polynomials*, Gordon and Breach, New York.

Christoffel E. B. (1858) Über die Gaussische Quadratur und eine Verallgemeinerung Derselben. *J. Reine Angew. Math.* **55**, 61.

Christoffel E. B. (1877) Sur une Classe Particulière de Fonctions Entières et de Fractions Continues. *Ann. Mat. Pura Appl. (2)* **8**, 1.

Clenshaw C. W. (1955) A Note on the Summation of Chebyshev Series, *Math. Tables Aids Comput.* **9**, 118.

Darboux G. (1878) Mémoire sur l'Approximation des Fonctions de Très-Grands Nombres et sur une Classe Étendue de Développements en Série. *J. Math. Pures Appl. (3)* **4**, 5.

Davis P. J. and Rabinowitz P. (1984) *Methods of Numerical Integration*, 2nd edition, Academic Press, San Diego.

Davison B. (1957) *Neutron Transport Theory*, Oxford University Press, London.

Dubrulle A., Martin R. S. and Wilkinson J. H. (1968) The Implicit QL Algorithm, *Numer. Math.* **12**, 377.

Engle, Jr. W. W. (1973) *A Users Manual for ANISN, a One Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering*, Report K-1693 (updated), Union Carbide, Nuclear Division.

Erdélyi A., Magnus W., Oberhettinger F. and Tricomi F. G. (1953) *Higher Transcendental Functions*, McGraw-Hill, New York.

Fejér L. (1933) Mechanische Quadraturen mit Positiven Cotesschen Zahlen. *Math Z.* **37**, 287.

Francis J. G. F. (1961) The Q-R Transformation: A Unitary Analogue to the L-R Transformation. I *Comput. J.* **4**, 265.

Francis J. G. F. (1962) The Q-R Transformation: A Unitary Analogue to the L-R Transformation. II *Comput. J.* **4**, 332.

Freud G. (1971) *Orthogonal Polynomials*, Pergamon, Oxford.

Galant D. (1971) An Implementation of Christoffel's Theorem in the Theory of Orthogonal Polynomials. *Math. Comp.* **25**, 111.

Garcia R. D. M. (1985) A Review of the Facile (F_N) Method in Particle Transport Theory. *Transp. Theory Stat. Phys.* **14**, 391.

Garcia R. D. M. and Ono S. (1999) Improved Discrete-Ordinates Calculations for an Approximate Model of Neutral Particle Transport in Ducts. *Nucl. Sci. Eng.*, accepted for publication.

Garcia R. D. M. and Siewert C. E. (1982) On the Dispersion Function in Particle Transport Theory. *Z. Angew. Math. Phys.* **33**, 801.

Garcia R. D. M. and Siewert C. E. (1989) On Discrete Spectrum Calculations in Radiative Transfer. *J. Quant. Spectrosc. Radiat. Transfer* **42**, 385.

Garcia R. D. M. and Siewert C. E. (1990) On Computing the Chandrasekhar Polynomials in High Order and High Degree. *J. Quant. Spectrosc. Radiat. Transfer* **43**, 201.

Garcia R. D. M., Siewert C. E. and Thomas Jr. J. R. (1994) F_N Method for Solving Transport Problems. *Trans. Am. Nucl. Soc* **71**, 212.

Garcia R. D. M. and Siewert C. E. (1998) The F_N Method in Atmospheric Radiative Transfer. *Int. J. Eng. Sci.* **36**, 1623.

Gautschi W. (1967) Computational Aspects of Three-Term Recurrence Relations. *SIAM Rev.* **9**, 24.

Gautschi W. (1968a) Construction of Gauss-Christoffel Quadrature Formulas. *Math. Comp.* **22**, 251.

Gautschi W. (1968b) Algorithm 331—Gaussian Quadrature Formulas. *Comm. ACM* **11**, 432.

Gautschi W. (1978) Questions of Numerical Condition Related to Polynomials. In *Recent Advances in Numerical Analysis* (C. de Boor and G. H. Golub, eds.), p. 45, Academic Press, New York.

Gautschi W. (1979) On Generating Gaussian Quadrature Rules. In *Numerische Integration* (G. Hämmerlin, ed.), p. 147, Birkhäuser, Basel.

Gautschi W. (1981) Minimal Solutions of Three-Term Recurrence Relations and Orthogonal Polynomials. *Math. Comp.* **36**, 547.

Gautschi W. (1982a) On Generating Orthogonal Polynomials. *SIAM J. Sci. Stat. Comput.* **3**, 289.

Gautschi W. (1982b) An Algorithmic Implementation of the Generalized Christoffel Theorem. In *Numerical Integration* (G. Hämmerlin, ed.), p. 89, Birkhäuser, Basel.

Gautschi W. (1984) On Some Orthogonal Polynomials of Interest in Theoretical Chemistry. *BIT* **24**, 473.

Gautschi W. (1985) Orthogonal Polynomials—Constructive Theory and Applications. *J. Comput. Applied Math.* **12&13**, 61.

Gautschi W. (1990) Computational Aspects of Orthogonal Polynomials. In *Orthogonal Polynomials: Theory and Practice* (P. Nevai, ed.), p. 181, Kluwer Academic Publishers, Dordrecht, The Netherlands.

Goldstein H. (1959) *Fundamental Aspects of Reactor Shielding*, Addison-Wesley, Reading, Mass.

Golub G. H. and Welsch J. H. (1969) Calculation of Gauss Quadrature Rules. *Math. Comp.* **23**, 221.

Hill T. R., Shultis J. K. and Mingle J. O. (1974) Numerical Evaluation of the Azimuthally Dependent Albedo Problem in Slab Geometry. *J. Comput. Phys.* **15**, 200.

Hochstrasser U. W. (1964) Orthogonal Polynomials. In *Handbook of Mathematical Functions* (M. Abramowitz and I. A. Stegun, eds.), p. 771, National Bureau of Standards, Washington, D.C.

İnönü E. (1970) Orthogonality of a Set of Polynomials Encountered in Neutron-Transport and Radiative-Transfer Theories. *J. Math. Phys.* **11**, 568.

Larsen E. W. (1984) A One-Dimensional Model for Three-Dimensional Transport in a Pipe. *Transp. Theory Stat. Phys.* **13**, 599.

Larsen E. W., Malvagi F. and Pomraning G. C. (1986) One-Dimensional Models for Neutral Particle Transport in Ducts. *Nucl. Sci. Eng.* **93**, 13.

Liou K.-N. (1980) *An Introduction to Atmospheric Radiation*, Academic Press, New York.

McCormick N. J. and Kuščer I. (1973) Singular Eigenfunction Expansions in Neutron Transport Theory. *Adv. Nucl. Sci. Technol.* **7**, 181.

McCormick N. J. and Veeder J. A. R. (1978) On the Inverse Problem of Transport Theory with Azimuthal Dependence. *J. Math. Phys.* **19**, 994.

McMahon D. R. A. and Shizgal B. (1985) Hot-Electron Zero-Field Mobility and Diffusion in Rare-Gas Moderators. *Phys. Rev. A* **31**, 1894.

Mika J. R. (1961) Neutron Transport with Anisotropic Scattering. *Nucl. Sci. Eng.* **11**, 415.

Mobley, C. D. (1994) *Light and Water: Radiative Transfer in Natural Waters*, Academic Press, San Diego.

Press W. H., Flannery B. P., Teukolsky S. A. and Vetterling W. T. (1986) *Numerical Recipes, the Art of Scientific Computing*, Cambridge University Press, Cambridge, UK.

Prinja A. K. and Pomraning G. C. (1984) A Statistical Model of Transport in a Vacuum. *Transp. Theory Stat. Phys.* **13**, 567.

Sack R. A. and Donovan A. F. (1972) An Algorithm for Gaussian Quadrature Given Modified Moments. *Numer. Math.* **18**, 465.

Selph W. E. (1973) Albedos, Ducts, and Voids. In *Reactor Shielding for Nuclear Engineers* (N. M. Schaeffer, ed.), p. 313, U.S. Atomic Energy Commission Office of Information Services, Washington, D.C.

Shizgal B. (1981a) A Gaussian Quadrature Procedure for Use in the Solution of the Boltzmann Equation and Related Problems. *J. Comput. Phys.* **41**, 309.

Shizgal B. (1981b) Nonequilibrium Time Dependent Theory of Hot Atom Reactions. III. Comparison with Estrup-Wolfgang Theory. *J. Chem. Phys.* **74**, 1401.

Shizgal B. (1983) Electron Thermalization in Gases. *J. Chem. Phys.* **78**, 5741.

Shizgal B. (1992) Spectral Theory and the Approach to Equilibrium in a Plasma. *Transp. Theory Stat. Phys.* **21**, 645.

Shizgal B. and Blackmore R. (1983) Eigenvalues of the Boltzmann Collision Operator for Binary Gases: Relaxation of Anisotropic Distributions. *Chem. Phys.* **77**, 417.

Shizgal B. and Blackmore R. (1984) A Discrete Ordinate Method of Solution of Linear Boundary Value and Eigenvalue Problems. *J. Comput. Phys.* **55**, 313.

Shizgal B. and Karplus M. (1971) Nonequilibrium Contribution to the Rate of Reaction. III. Isothermal Multicomponent Systems. *J. Chem. Phys.* **54**, 4357.

Shizgal B., Lindenfeld M. J. and Reeves R. (1981) Eigenvalues of the Boltzmann Collision Operator for Binary Gases: Mass Dependence. *Chem. Phys.* **56**, 249.

Shizgal B. and McMahon D. R. A. (1984) Electric Distribution Functions and Thermalization Times in Inert Gas Moderators. *J. Phys. Chem.* **88**, 4854.

Shizgal B. and McMahon D. R. A. (1985) Electric Field Dependence of Transient Electron Transport Properties in Rare-Gas Moderators. *Phys. Rev. A* **32**, 3669.

Shohat J. (1934) *Théorie Générale des Polynomes Orthogonaux de Tchebichef.* Mémorial des Sciences Mathématiques, Vol. 66, Gauthier-Villars, Paris.

Siewert C. E. and Benoist P. (1979) The F_N Method in Neutron-Transport Theory. Part I: Theory and Applications. *Nucl. Sci. Eng.* **69**, 156.

Siewert C. E. and McCormick N. J. (1997) Some Identities for Chandrasekhar Polynomials. *J. Quant. Spectrosc. Radiat. Transfer* **57**, 399.

Smith B. T., Boyle J. M., Dongarra J. J., Garbow B. S., Ikebe Y., Klema V. C. and Moler C. B. (1976) *Matrix Eigensystem Routines—EISPACK Guide*, 2nd edition, Springer-Verlag, Berlin.

Stiefel E. L. (1958) Kernel Polynomials in Linear Algebra and their Numerical Applications. In *Further Contributions to the Solution of Simultaneous Linear Equations and the Determination of Eigenvalues*, NBS Appl. Math. Series, Vol. 49, p. 1, National Bureau of Standards, Washington, D.C.

Stieltjes T. J. (1884) Quelques Recherches sur la Théorie des Quadratures Dites Mécaniques. *Ann. Sci. École Norm. Sup. (3)* **1**, 409.

Stroud A. H. and Secrest D. (1966) *Gaussian Quadrature Formulas.* Prentice-Hall, Englewood Cliffs, N.J.

Szegö G. (1939) *Orthogonal Polynomials*, American Mathematical Society, Providence, R.I.

Uvarov V. B. (1959) Relation between Polynomials Orthogonal with Different Weights. *Dokl. Akad. Nauk SSSR* **126**, 33.

Uvarov V. B. (1969) The Connection between Systems of Polynomials that Are Orthogonal with Respect to Different Distribution Functions. *U.S.S.R. Computational Math. and Phys.* **9**, 25.

Wheeler J. C. (1974) Modified Moments and Gaussian Quadrature. *Rocky Mountain J. Math.* **4**, 287.

Wheeler J. C. (1984) Modified Moments and Continued Fraction Coefficients for the Diatomic Linear Chain. *J. Chem. Phys.* **80**, 472.

Wick, G. C. (1943) Über ebene Diffusionsprobleme. *Z. Phys.* **121**, 702.