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On the Generation of Orthogonal Polynomials Using Asymptotic Methods for Recurrence Coefficients

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A set of orthogonal polynomials is defined by specifying an interval and a weight function. Any such set of polynomials satisfies a three term recurrence relation with coefficients α_n and β_n, which in turn satisfy coupled recurrence relations. If the polynomials do not belong to the set of *classical* polynomials, these recurrence relations are generally numerically unstable. In this paper, we consider the generation of several sets of orthogonal polynomials that are useful in the solution of different physical problems. We construct recurrence relations for the coefficients in the three term recurrence relations of these polynomials and study their numerical instability. Divergent asymptotic series for the recurrence coefficients are derived and used to obtain accurate approximations through the use of direct summation or continued fractions. A comparison of these approximate recurrence coefficients is made with the accurate values obtained with the use of multiple precision arithmetic. © 1993 Academic Press, Inc.

1. INTRODUCTION

Classical orthogonal polynomials have been used as basis functions in the solution of a large number of physical problems described by differential and/or integral equations. The choice of basis set is dictated by the interval over which the problem is defined, as well as the anticipated behaviour of the solutions which suggest the form of the weight function. In many applications, it is preferable to consider a weight function which leads to a set of *nonclassical* polynomials. Several years ago Shizgal [1] constructed the polynomials orthogonal with weight function $w(x) = x^2 e^{-x^2}$ on the interval $[0, \infty]$ and demonstrated the way in which this basis set greatly accelerated the convergence of the eigenvalues of the Lorentz Fokker–Planck operator relative to the use of Laguerre polynomials. The Laguerre polynomials are generated with the weight function $w(x) = e^{-x}$ on the interval $[0, \infty]$. Other examples of nonclassical polynomials include the sets generated with weight functions $w(x) = e^{-ax^4/2 + bx^2}$ on the interval $[-\infty, \infty]$ [2], $w(x) = x^2 e^{-a(x-x_0)^2}$ on $[0, \infty]$ [3], and $w(x) = x^2 e^{-ax^4}$ on $[0, \infty]$ for use in electron transport calculations. It is well known that the generation of nonclassical polynomials basis sets is numerically unstable [4]. A more recent discussion of the computational aspects of orthogonal polynomials has been given by Gautschi [5], where several other nonclassical polynomials are presented.

These sets of orthogonal polynomials also serve to define a quadrature procedure such that integrals over the weight function are given by

$$\int_0^{\infty} w(x) f(x)\, dx \approx \sum_{i=1}^{N} w_i f(x_i), \tag{1}$$

where the calculation of the weights and points, w_i, x_i, have been described elsewhere [6]. The points, x_i, are the roots of the polynomial of order N. The solution of integral and/or differential equations can also be formulated in terms of a discretization of the unknown function, that is, by the values of the function at the quadrature points rather than by the explicit expansion in the basis set. This is the basis for the quadrature discretization method (QDM) developed by Shizgal and Blackmore [7] and an analogous procedure referred to as the discrete variable representation (DVR) by Light and co-workers [8].

The QDM and the DVR are similar to collocation methods and belong to the large class of spectral methods in numerical analysis [9]. However, spectral methods are generally restricted to the use of Chebyshev polynomials or Fourier series as basis set expansions. There is considerable interest in using spectral methods based on other polynomials. The present paper is directed towards this objective. In Section 2, we discuss the derivation of the recurrence relations for the coefficients in the three term recurrence relations for several different weight functions. We derive asymptotic expansions in Section 3 so as to generate approximate but accurate values for the recurrence coefficients. The leading behavior of the asymptotic expansions are used to analyse the stability of these recurrence relations in Section 4. Summation of asymptotic series and numerical results are discussed in Section 5. A summary of our methods and results is presented in Section 6.

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2. THREE TERM RECURRENCE COEFFICIENTS

Any set of orthogonal polynomials of the form discussed in the introduction satisfy a three term recurrence relation of the form,

$$Q_{n+1}(x)=(x-\alpha_n)\,Q_n(x)-\beta_n Q_{n-1}, \qquad (2)$$

where $Q_0=1$. The polynomials generated with Eq. (2) are not normalized to 1. The normalized polynomials $P_n=Q_n/\sqrt{\gamma_n}$ satisfy the recurrence relation

$$xP_n(x)=\sqrt{\beta_{n+1}}\,P_{n+1}(x)+\alpha_n P_n(x)+\sqrt{\beta_n}\,P_{n-1}(x), \qquad (3)$$

where the normalization factors are given by

$$\gamma_n=\langle Q_n^2\rangle. \qquad (4)$$

The symbol $\langle\ \rangle$ denotes the integration over x with the weight function and is referred to as the average over x. The coefficients β_n and α_n are given by

$$\beta_n=\gamma_n/\gamma_{n-1} \qquad (5)$$

and

$$\alpha_n=\langle xP_n^2\rangle. \qquad (6)$$

The sections that follow outline the results obtained for three different weight functions. The first two have been discussed previously, whereas the results for the third are new.

2a. *Speed Polynomials*

Many problems in kinetic theory involve the evaluation of averages over a Maxwellian distribution function $f^M(c)$, where c is the particle speed. The equilibrium average value of a function $F(c)$ is given by

$$\bar{F}=\int f^M(c)\,F(c)\,dc$$
$$=\frac{4}{\sqrt{\pi}}\int_0^\infty e^{-x^2}x^2F(x)\,dx, \qquad (7)$$

where $f^M(c)=(m/2\pi kT)^{3/2}\exp(-mc^2/2kT)$, m is the mass, and $x=(m/2kT)^{1/2}c$ is the dimensionless speed. In an earlier paper, Shizgal [10] developed a Gaussian quadrature procedure for integrals of this type with the weight function $w(x)=x^p\exp(-x^2)$ on the interval $[0,\infty]$ and applied the results to the solution of the Boltzmann and/or Fokker–Planck equations [2]. For this weight function, the coefficients α_n, β_n which appear in the three term recurrence relation (Eq. (2)) satisfy the two recurrence relations,

$$\beta_{n+1}+\alpha_n^2+\beta_n=n+(p+1)/2 \qquad (8)$$

and

$$(n+1)(n+p+1)=4\beta_{n+1}[\alpha_n(\alpha_n+\alpha_{n+1})+\beta_n+\tfrac{1}{2}]. \qquad (9)$$

which are numerically unstable. With each iteration, a significant figure is lost so that in double precision these recurrence relations generate only 10–13 polynomials depending on the desired accuracy. Shizgal [10] employed extended precision arithmetic to generate the recurrence coefficients to high order (~ 100), and hence the polynomials and the associated quadrature weights and points to at least 16 significant figures.

2b. *Bimode Polynomials*

The Fokker–Planck equation with nonlinear drift and diffusion terms has been employed to describe the time evolution of many non-equilibrium systems in physics, chemistry, and biology [11]. In some situations the final equilibrium distribution function is bimodal. Blackmore and Shizgal [2] found that the weight function $w(x)=\exp(-ax^4/2+bx^2)$, defined on the interval $[-\infty,\infty]$, arises naturally in such problems. For this choice of weight function and interval, $\alpha_n=0$ and the β_n coeffecients satisfy the recurrence relation

$$\beta_{n+2}=\frac{n+1}{2a\beta_{n+1}}+\frac{b}{a}-\beta_{n+1}-\beta_n \qquad (10)$$

with $\beta_0=0$.

2c. *Druyvesteyn Polynomials*

At high electric field strength, the steady state electron velocity distribution of electrons dilutely dispersed in a background gas of atoms is given by the Druyvesteyn distribution function [12], provided that the electron–atom momentum transfer cross section is constant. This distribution function has the form $x^2\exp(-ax^4)$, where x is the reduced speed of the electrons. We expect that a quadrature method based on a weight function of this form will prove useful in the solution of electron transport problems. Since the derivation of the recurrence relations for this weight function has not previously been provided, we briefly outline the steps involved. The method closely follows that used by Shizgal [10].

We consider the weight function $w(x)=x^p\exp(-ax^4)$

defined on the interval $[0, \infty]$, for $p=0, 1, 2, \ldots$. The normalized polynomial $P_n(x)$ can be written as

$$P_n(x)=\frac{x^n}{\gamma_n^{1/2}}+\cdots \tag{11}$$

so that

$$xP_n'(x)=nP_n(x)+S(x), \tag{12}$$

where $S(x)$ is orthogonal to $P_n(x)$. Hence we obtain the identity

$$n=\langle xP_nP_n'\rangle. \tag{13}$$

If an integration by parts is performed on Eq. (13) and the identity

$$w'(x)=\frac{pw}{x}-4ax^3w \tag{14}$$

is employed, we obtain

$$2n+1+p=4a\langle x^4P_n^2\rangle. \tag{15}$$

With repeated application of Eq. (3) to the right-hand side of Eq. (15) and use of the orthogonality of the polynomials, we obtain the recurrence relation

$$\begin{aligned}2n+1+p=4a[&\beta_{n+1}^2+\beta_{n+1}\beta_{n+2}\\&+\beta_{n+1}\alpha_{n+1}^2+3\alpha_n^2\beta_{n+1}+3\alpha_n^2\beta_n\\&+\alpha_n^4+\beta_n^2+\beta_n\alpha_{n-1}^2+\beta_n\beta_{n-1}+2\alpha_n\alpha_{n+1}\beta_{n+1}\\&+2\alpha_n\alpha_{n-1}\beta_n+2\beta_n\beta_{n+1}].\end{aligned} \tag{16}$$

To obtain another recurrence relation we start with the Christoffel–Darboux identity [6], given by

$$\sum_{k=0}^{n}P_k^2=\sqrt{\beta_{n+1}}\,[P_{n+1}'P_n-P_{n+1}P_n']. \tag{17}$$

Multiplying both sides of Eq. (17) by $xw(x)$ and integrating, we find

$$\sum_{k=0}^{n}\alpha_k=\sqrt{\beta_{n+1}}\,\langle xP_{n+1}'P_n\rangle, \tag{18}$$

where we have used the fact that P_{n+1} is orthogonal to P_n'. Integrating the right-hand side of Eq. (18) by parts and using Eq. (14) we find

$$\sum_{k=0}^{n}\alpha_k=4a\sqrt{\beta_{n+1}}\,\langle x^4P_{n+1}P_n\rangle. \tag{19}$$

With repeated application of Eq. (3) we obtain a second recurrence relation,

$$\begin{aligned}\sum_{k=0}^{n}\alpha_k=4a\beta_{n+1}[&\alpha_{n+2}\beta_{n+2}+2\alpha_{n+1}\beta_{n+2}\\&+\alpha_n\beta_{n+2}+2\alpha_{n+1}\beta_{n+1}+\alpha_{n+1}\beta_n\\&+2\alpha_n\beta_{n+1}+2\alpha_n\beta_n+\alpha_{n-1}\beta_n+\alpha_{n+1}^3\\&+\alpha_n^3+\alpha_n\alpha_{n+1}^2+\alpha_n^2\alpha_{n+1}].\end{aligned} \tag{20}$$

Equations (16) and (20) are the desired recurrence relations. They are third-order finite difference equations and require six initial values $(\alpha_0, \alpha_1, \alpha_2, \beta_1, \beta_2, \beta_3)$. These initial values are easily evaluated in terms of the moments $\mu_n=\langle x^n\rangle$, using Eqs. (3)–(6).

3. ASYMPTOTIC EXPANSIONS

Asymptotic properties of orthogonal polynomials (particularly those associated with exponential weight functions) have been investigated by Nevai *et al.* [13], Magnus [14], Lew and Quarles [15], and Van Assche [16]. Langhoff [17] also discusses asymptotic series to approximate recurrence coefficients. The asymptotic techniques we discuss here are similar to techniques described by Lew and Quarles, and Magnus.

For all the weight functions discussed in Section 2, the recurrence relations for the α_n and β_n coefficients are numerically unstable. Using double precision arithmetic with approximately 16-digit accuracy, we were only able to generate about 10 α_n and β_n coefficients for the Druyvesteyn and speed polynomials, and approximately 25 for the bimode polynomials. Ideally we would like to be able to calculate an *arbitrary* number of α_n and β_n coefficients to high precision. Here we investigate the use of asymptotic expansions to obtain approximate but accurate values for α_n and β_n as a function of n.

3a. *Speed Polynomials*

The first step in deriving an asymptotic series solution is to find the leading behavior, that is, the first term in the expansion. In all the cases described in Section 2, the α_n and β_n coefficients are all positive and approach infinity as $n\to\infty$. This suggests that we write

$$\alpha_n=n^r\tilde{\alpha}_n, \quad \beta_n=n^s\tilde{\beta}_n, \tag{21}$$

where the quantities $\tilde{\alpha}_n$ and $\tilde{\beta}_n$ approach positive constants A and B, respectively, as $n\to\infty$. Thus $\alpha_n\sim An^r$ and $\beta_n\sim Bn^s$ as $n\to\infty$, where r and s are unknown positive constants and $\sim$ means *asymptotic to.* Substituting these asymptotic forms into the recurrence relations Eqs. (8) and (9), we obtain the two equations

$$2Bn^s + A^2 n^{2r} = n \tag{22}$$

$$n^2 = 4Bn^s(2A^2 n^{2r} + Bn^s). \tag{23}$$

We require that these equations hold for all $n > 0$ so that $s = 1$ and $r = \frac{1}{2}$. The coefficients A and B satisfy the two equations

$$2B + A^2 = 1 \tag{24}$$

$$4B(2A^2 + B) = 1. \tag{25}$$

There are two possible solutions, namely $A = 0$, $B = \frac{1}{2}$ or $A = \sqrt{2/3}$, $B = \frac{1}{6}$. However, α_n and β_n are positive for all n, so A and B must both be positive. Thus $A = \sqrt{2/3}$, $B = \frac{1}{6}$, and the leading behavior is given by

$$\alpha_n \sim \sqrt{2n/3}, \quad \beta_n \sim n/6. \tag{26}$$

We now write the asymptotic expansions of the coefficients $\tilde{\alpha}_n$ and $\tilde{\beta}_n$ in the form

$$\tilde{\alpha}_n = \sum_{k=0}^{\infty} a_k \varepsilon^k, \quad \tilde{\beta}_n = \sum_{k=0}^{\infty} b_k \varepsilon^k. \tag{27}$$

Here $\varepsilon = 1/n^z$, z is an as yet undetermined positive constant, and the first terms in the series are given by $a_0 = A$ and $b_0 = B$. In general, these are *divergent* asymptotic expansions in the small parameter ε.

In general, the recurrence relations for the α_n and β_n coefficients are coupled, nonlinear finite difference equations. Once we have found the leading behavior, substitution of Eq. (27) leads to a pair of linear equations for the a_k and b_k expansion coefficients at each order (k) of the expansion. These equations are then easily decoupled to obtain explicit expressions for the a_k and b_k coefficients in terms of the set of lower order coefficients, that is $\{a_i, b_i\}_{i<k}$. Note that for fixed order k, the asymptotic expansions become *more* accurate as $n \to \infty$. This is in contrast to other approximation methods [4, 18, 19], where the accuracy rapidly *decreases* with increasing n.

Substituting Eq. (21) (with $s = 1$ and $r = \frac{1}{2}$) into Eqs. (8) and (9), we obtain

$$(n+1)\tilde{\beta}_{n+1} + n\tilde{\alpha}_n^2 + n\tilde{\beta}_n = n + (p+1)/2 \tag{28}$$

$$(n+p+1) = 4\tilde{\beta}_{n+1}[\sqrt{n}\,\tilde{\alpha}_n(\sqrt{n}\,\tilde{\alpha}_n + \sqrt{n+1}\,\tilde{\alpha}_{n+1}) + n\tilde{\beta}_n + 1/2]. \tag{29}$$

We next determine the value of z. Divide both sides of Eqs. (28) and (29) by n and note that all coefficients can be expanded as power series in $\varepsilon = 1/n^z$, where $z = 1$. Replacing $1/n$ by ε, we obtain

$$(1+\varepsilon)\tilde{\beta}_{n+1} + \tilde{\alpha}_n^2 + \tilde{\beta}_n = 1 + [(p+1)/2]\varepsilon \tag{30}$$

$$[1 + (p+1)\varepsilon] = 4\tilde{\beta}_{n+1}[\tilde{\alpha}_n^2 + (1+\varepsilon)^{1/2}\tilde{\alpha}_n\tilde{\alpha}_{n+1} + \tilde{\beta}_n + (1/2)\varepsilon]. \tag{31}$$

In order to evaluate the a_k, b_k coefficients in the asymptotic series for $\tilde{\alpha}_n$ and $\tilde{\beta}_n$, we write Eqs. (30) and (31) as power series in ε. Substituting $1/(n+1) = \varepsilon/(1+\varepsilon)$ into $\tilde{\beta}_{n+1} = \sum_{k=0}^{\infty} b_k(1/(n+1)^k)$ (and similarly for $\tilde{\alpha}_{n+1}$), we obtain

$$\tilde{\alpha}_{n+1} = \sum_{k=0}^{\infty} a_k \varepsilon^k (1+\varepsilon)^{-k} \tag{32}$$

$$\tilde{\beta}_{n+1} = \sum_{k=0}^{\infty} b_k \varepsilon^k (1+\varepsilon)^{-k}. \tag{33}$$

Finally we substitute Eqs. (32) and (33) into Eqs. (30) and (31), expand all terms in powers of ε, and equate coefficients of equal powers of ε.

To illustrate the procedure we derive the equations for the coefficients a_1 and b_1. Expanding Eqs. (32) and (33) in powers of ε and keeping only terms of order ε or lower, we obtain

$$\tilde{\alpha}_{n+1} = \tilde{\alpha}_n \simeq a_0 + a_1\varepsilon, \tag{34}$$

and similarly for $\tilde{\beta}_{n+1}$ and $\tilde{\beta}_n$. The next step is to substitute these expressions into Eqs. (30) and (31) and expand all other terms in powers of ε, retaining only terms of order ε or lower. Finally, we substitute the known values of a_0 and b_0 and equate the coefficients of ε to obtain the two equations

$$2b_1 + (2\sqrt{2/3})\,a_1 = p/2 + 1/3 \tag{35}$$

$$(8/3\sqrt{2/3})\,a_1 + (20/3)\,b_1 = p + 4/9. \tag{36}$$

The solution of these equations gives $a_1 = (\frac{3}{2})^{1/2}((p+1)/6)$ and $b_1 = p/12$. We find in analogous fashion that the next terms are given by $a_2 = (\frac{3}{2})^{1/2}[(6p^2 - 6p - 5)/144]$ and $b_2 = [(2 - 9p^2)/144]$. In most cases it is easy to obtain the first few a_k and b_k coefficients analytically, but as the order k increases, the number of terms one must keep track of increases rapidly. In Section 5 we discuss two methods for obtaining the higher order coefficients.

3b. *Bimode Polynomials*

The derivation of the asymptotic series for the coefficients β_n for the bimode polynomials is simpler than the derivation for the speed polynomials since there is now only one recurrence relation. Rewriting the recurrence relation Eq. (10) in the form

$$\beta_{n+2}\beta_{n+1} = \frac{n+1}{2a} + \frac{b}{a}\beta_{n+1} - \beta_{n+1}^2 - \beta_{n+1}\beta_n \quad (37)$$

and substituting $\beta_n \sim Bn^s$, we find $B = b_0 = (b/a)(\mu/3)^{1/2}$ and $s = \frac{1}{2}$, where $\mu = a/(2b^2)$. With the leading behavior, we can systematically determine the coefficients in the asymptotic series expansion. However, the presence of the term $(b/a)\,\beta_{n+1}$ in Eq. (37) requires that the series expansion be in powers of $\varepsilon = n^{-1/2}$, instead of $\varepsilon = n^{-1}$, as in the case of speed polynomials. From this point on, the procedure for calculating higher order terms in the series expansion is exactly as in the case of speed polynomials. The first six terms are $b_0 = (b/a)\sqrt{\mu/3}$, $b_1 = b/(6a)$, $b_2 = b/(24a\sqrt{3\mu})$, $b_3 = 0$, $b_4 = b(48\mu^2 - 1)/(1152a\mu^2\sqrt{\mu/3})$, $b_5 = b/(144a)$.

3c. *Druyvesteyn Polynomials*

The α_n and β_n coefficients are given by Eqs. (16) and (20). The coefficients α_n scale as $a^{-1/4}$ and the coefficients β_n scale as $a^{-1/2}$, where "a" is the constant which appears in the weight function $w(x) = x^p \exp(-ax^4)$. In order to simplify the algebra we henceforth set $a = 1$. The calculation of the coefficients in the asymptotic series for the α_n and β_n coefficients is made more complicated by the term $\sum_{k=0}^{n} \alpha_k$ appearing in Eq. (20). Since α_n has an asymptotic expansion of the form given by Eq. (21), that is,

$$\alpha_n \sim a_0 n^r + a_1 n^{r-1} + a_2 n^{r-2} + \cdots, \quad (38)$$

then the $\sum_{k=0}^{n} \alpha_k$ can be evaluated approximately by converting the sum to an integral and we anticipate the sum to have the asymptotic form

$$\sum_{k=0}^{n} \alpha_k \sim h_0 n^{r+1} + h_1 n^r + h_2 n^{r-1} + \cdots. \quad (39)$$

The coefficients $h_0, h_1, \ldots$ are determined by applying the general Euler–Maclaurin summation formula valid for $n \to \infty$ [20], given by

$$\sum_{k=0}^{n} f(k) \sim \frac{1}{2} f(n) + \int_0^n f(t)\,dt + C + \sum_{j=1}^{\infty} (-1)^{j+1} \frac{B_{j+1}}{(j+1)!} f^{(j)}(n) \quad (40)$$

to each term in the series

$$\sum_{k=0}^{n} \alpha_k \sim a_0 \sum_{k=0}^{n} k^r + a_1 \sum_{k=1}^{n} k^{r-1} + a_2 \sum_{k=1}^{n} k^{r-2} + \cdots. \quad (41)$$

In Eq. (41), C is a constant [20] and B_j is the jth Bernoulli number for which the lowest order numbers are $B_0 = 1$, $B_1 = -\frac{1}{2}$, $B_2 = \frac{1}{6}$, $B_3 = 0$, $B_4 = -\frac{1}{30}$, etc. We evaluate the $\sum_k$ in each term of Eq. (41) with the summation formula Eq. (40). For example, the first summation on the right-hand side of Eq. (40) is given by

$$\sum_{k=0}^{n} \alpha_k \sim \frac{n^{5/4}}{5/4} + \frac{n^{1/4}}{2} + C_0 + \frac{n^{-3/4}}{48} + \cdots. \quad (42)$$

With this result in Eq. (41) we obtain, by comparison with Eq. (39), that $h_0 n^{r+1} = a_0 n^{r+1}/(r+1)$. The coefficients α_n and β_n in the asymptotic expansion are evaluated as for the other polynomials with Eqs. (16) and (20) and the asymptotic result Eq. (41). To lowest order this procedure gives (with $a = 1$) $a_0 = A = 2/(140)^{1/4}$, $b_0 = B = 1/(140)^{1/2}$ and $r = 1/4$, $s = 1/2$. This gives the leading behavior in the asymptotic expansions for α_n and β_n.

To evaluate the higher order terms, we obtain similar expressions for the terms $\sum_{k=1}^{n} k^{r-1}$, etc. to obtain explicit expressions for the coefficients $h_0, h_1, \ldots$. After some algebra, we find $h_1 = a_0/2 + 4a_1$, $h_2 = a_0/48 + a_1/2 - 4a_2/3$, etc. We have set to zero the constant terms $C_T = a_0 C_0 + a_1 C_1 + \cdots$ that result from the Euler–Maclaurin summation expression for $\sum_{k=0}^{n} \alpha_k$. This is reasonable since we assume that α_n and β_n have the form given in Eq. (21), where $\tilde{\alpha}_n$ and $\tilde{\beta}_n$ approach constants as $n \to \infty$. The choice $C_T = 0$ is consistent with this behavior. This choice is also justified by the fact that comparison of the asymptotic solutions for α_n and β_n with the exact results, discussed in Section 5, indicates that the error in the asymptotic results decreases rapidly with increasing n.

4. STABILITY ANALYSIS

The techniques of Section 2 when applied to *classical* orthogonal polynomials (e.g., Laguerre or Hermite) yield simple analytic results for α_n and β_n versus n. However, for nonclassical polynomials the *same* techniques yield nonlinear recurrence relations for α_n and β_n which are numerically unstable. In this section we use the asymptotic solutions described in Section 3 to understand the nature of this numerical instability. The instability is quite dramatic and we usually find that approximately one digit of accuracy is lost in each iteration. To understand this [19], we consider a recurrence relation of the form

$$\alpha_{n+1} = f(\alpha_n, \beta_n), \quad \beta_{n+1} = g(\alpha_n, \beta_n). \quad (43)$$

The recurrence relations derived in Section 2 are generally more complicated than this, but the method we describe can easily be generalized. Suppose that the nth iterates are given by

$$\alpha_n = \alpha_n^{\text{exact}} + \delta_n, \quad \beta_n = \beta_n^{\text{exact}} + \varepsilon_n, \tag{44}$$

where δ_n and ε_n are the errors in α_n and β_n. Assuming $\delta_n \ll \alpha_n^{\text{exact}}$ and $\varepsilon_n \ll \beta_n^{\text{exact}}$, we then have

$$\begin{aligned} \alpha_{n+1} &= f(\alpha_n^{\text{exact}} + \delta_n, \beta_n^{\text{exact}} + \varepsilon_n) \\ &\simeq f(\alpha_n^{\text{exact}}, \beta_n^{\text{exact}}) + \frac{\partial f}{\partial \alpha_n^{\text{exact}}} \delta_n + \frac{\partial f}{\partial \beta_n^{\text{exact}}} \varepsilon_n \\ &= \alpha_{n+1}^{\text{exact}} + \frac{\partial f}{\partial \alpha_n^{\text{exact}}} \delta_n + \frac{\partial f}{\partial \beta_n^{\text{exact}}} \varepsilon_n \end{aligned} \tag{45}$$

and similarly for β_{n+1}. The relative error in α_n is given by $\delta_n/\alpha_n^{\text{exact}}$ and the relative error in α_{n+1} is given by $[(\partial f/\partial \alpha_n^{\text{exact}})\, \delta_n + (\partial f/\partial \beta_n^{\text{exact}})\, \varepsilon_n]/\alpha_{n+1}^{\text{exact}}$. Thus the relative error increases if

$$\left| \frac{[(\partial f/\partial \alpha_n^{\text{exact}})\, \delta_n + (\partial f/\partial \beta_n^{\text{exact}})\, \varepsilon_n]}{\alpha_{n+1}^{\text{exact}}} \right| > \left| \frac{\delta_n}{\alpha_n^{\text{exact}}} \right|. \tag{46}$$

An approximate condition for error growth in α_{n+1} is then

$$\left| \frac{\partial f}{\partial \alpha_n^{\text{exact}}} \right| > 1 \quad \text{or} \quad \left| \frac{\partial f}{\partial \beta_n^{\text{exact}}} \right| > 1. \tag{47}$$

(A similar analysis applies for β_{n+1}.) If the magnitudes of any of these partial derivatives are larger than 1, then, even if all calculations are done in infinite precision arithmetic but the starting values α_0, β_0 have finite precision, the coefficients α_n and β_n will eventually become inaccurate as n increases.

To decide whether a recurrence relation is numerically unstable, it is necessary to have an estimate of the coefficients α_n and β_n for large n. We presented a method for obtaining such estimates in Section 3. We use the results of Section 3 to illustrate the numerical instability that occurs in the calculation of the coefficients α_n and β_n for the weight function $w(x) = x^p e^{-x^2}$ $(p = 0, 1, 2, ...)$ on the interval $[0, \infty]$, i.e., the speed polynomials. The recurrence relations are given by Eqs. (8) and (9), which can be rearranged in the form of Eq. (43). The function $g(\alpha_n, \beta_n)$ is easily obtained from Eq. (8) and we have that (for large n)

$$\frac{\partial g}{\partial \alpha_n^{\text{exact}}} = 2\alpha_n^{\text{exact}} \simeq 2\sqrt{2n/3}, \tag{48}$$

where the asymptotic result, Eq. (26) has been used, and

$$\frac{\partial g}{\partial \beta_n^{\text{exact}}} = -1. \tag{49}$$

The function $f(\alpha_n, \beta_n)$ is more complicated and is obtained by solving Eq. (9) for α_{n+1} and substituting for β_{n+1} from Eq. (8). The derivative of $f(\alpha_n, \beta_n)$ with respect to α_n can be evaluated, and with the asymptotic result, Eq. (26), we find (for large n)

$$\frac{\partial f}{\partial \alpha_n^{\text{exact}}} \simeq 14.75 \tag{50}$$

and

$$\frac{\partial f}{\partial \beta_n^{\text{exact}}} \simeq 9\sqrt{3/(2n)}. \tag{51}$$

The two terms which are greater than 1 (in absolute value) cause the numerical instability. Note that the term $\partial g/\partial \alpha_n^{\text{exact}} \simeq 2\sqrt{2n/3}$ is greater than one even for small n. Thus these recurrence relations are numerically unstable for *all n*. Similar results hold for the bimode and Druyvesteyn polynomials. It is interesting to note that, although linear recurrence relations which are unstable in the forward direction are stable in the backward direction [19], this does not hold in general for nonlinear recurrence relations. In particular, suppose that we calculate a very accurate estimate for α_n, β_n for $n \gg 1$, using the asymptotic methods discussed here. Then, for all three weight functions discussed in Section 2, backward iteration of the recurrence relations for α_n and β_n is numerically unstable.

5. NUMERICAL RESULTS

The main objective of the present paper is the development of an accurate computational method to calculate the coefficients α_n and β_n in the three term recurrence relation for nonclassical polynomials without resorting to multiple precision arithmetic. The ultimate objective is to be able to generate, accurately and efficiently, quadrature weights and points for arbitrary weight functions parametrized by physical quanties. In the preceeding sections, we have presented an asymptotic representation of these coefficients, Eqs. (21) and (27) for three different nonclassical polynomials. In the present section, we compare the results obtained for different orders in the asymptotic expansions with exact results obtained with multiple precision arithmetic.

The direct summation of the asymptotic series may not be useful beyond the first few terms since the coefficients eventually increase rapidly with increasing k. Alternatively, one can express the kth approximant to the asymptotic series in the form of a ratio of lower degree polynomials (Padé approximants) or in the form of a continued fraction, as described in Bender and Orszag [20]. Both Padé approximants and continued fractions may converge, where an ordinary power series diverges. However, continued fractions are more convenient for numerical calculations [20]. Given the kth order continued fraction approximant for an arbitrary function $f(x)$

$$f^{(k)}(x)=c_0/(1+c_1x/(1+c_2x/(1+\cdots c_{k-1}x/(1+c_kx)))\cdots). \tag{52}$$

the $(k+1)$th-order continued fraction approximant is obtained from the kth-order approximant by replacing c_k by $c_k/(1+c_{k+1}x)$. This is not the case for Padé approximants. The Padé approximant of order $k=l+m$, $f^{(l)}_{(m)}(x)$ is defined by

$$f^{(l)}_{(m)}(x)=\frac{r_0+r_1x+r_2x^2+\cdots+r_lx^l}{s_0+s_1x+s_2x^2+\cdots+s_mx^m}. \tag{53}$$

and calculation of the next order approximant $f^{(l+1)}_{(m)}(x)$ requires, in addition to the added coefficient r_{l+1}, the recalculation of all the lower order coefficients $r_0, s_0, r_1, s_1, ..., r_l, s_l$. For this reason we used continued fractions instead of Padé approximants to sum the asymptotic series.

We calculated the continued fraction coefficients $c_0, c_1, ...$ and evaluated the continued fraction approximants using standard algorithms [20]. The continued fraction approximants should be more accurate than the corresponding asymptotic series for large k, since the asymptotic series coefficients diverge as $k\to\infty$. In practice, we found that for $k\leqslant 8$ there was usually little difference in accuracy between the continued fraction and series approximations.

For each of the three weight functions discussed in this paper, we were able to calculate the first few coefficients $\{a_k, b_k\}$ in the asymptotic series analytically. However, as k increases the analytic calculations become quite tedious so we obtained the higher order coefficients numerically. For the speed and bimode polynomials we were able to obtain the first 8–10 asymptotic series coefficients to acceptable accuracy. Beyond $k\simeq 10$, roundoff errors accumulate so that higher order coefficients are inaccurate [21]. A useful alternate method is to use a symbolic manipulation program such as Macsyma or SMP to calculate *analytical* expressions for the $\{a_k, b_k\}$ as functions of k and any other parameters which might appear in the recurrence relations (e.g., p in the speed polynomials).

We also calculated the corresponding continued fraction coefficients $c_0, c_1, ..., c_8$ and evaluated the continued fraction approximants using standard algorithms described in [20] for each of the three polynomials. We calculated the "exact" coefficients α_n and β_n from the recurrence relations using multiple precision arithmetic and used these results to calculate the relative error in the continued fraction approximants for each of the three polynomials. Table I gives the lower order coefficients a_k and b_k in the asymptotic series expansions for α_n and β_n for the speed polynomials

TABLE I

Asymptotic Series Coefficients a_k and b_k for the Speed Polynomials with $p=2$

k	a_k	b_k
0	8.1649(−1)[a]	1.6666(−1)
1	6.1237(−1)	1.6666(−1)
2	5.9536(−2)	−2.3611(−1)
3	−4.7841(−1)	2.3611(−1)
4	9.8212(−1)	−1.5639(−1)
5	−1.5644(0)	−2.6041(−3)
6	1.8931(0)	2.9406(−1)
7	−6.3172(−1)	−8.2333(−1)
8	−6.8526(0)	1.9374(0)

[a] (n) ≡ × 10^n.

(with $p=2$). Figure 1 shows the logarithm of the relative error in α_n as a function of n and k (the order of the approximant) for the speed polynomials. Even though we can accurately calculate the continued fraction approximants only to order $k\simeq 8$, the coefficients α_n and β_n are very accurate for $n\geqslant 10$. For $n\leqslant 10$ one can solve the recurrence relations without recourse to multiple precision arithmetic. In this way one can obtain an approximate set $\{\alpha_n, \beta_n\}$ for all n to better than eight digits of accuracy.

Table II gives the lower order coefficients b_k for the bimode polynomials for β_n for the choice $a=b=2$. Figure 2 shows the logarithm of the relative error in β_n as a function of n and k. As for the speed polynomials, we can obtain the β_n coefficients to ~8-digit accuracy for all n by using double precision in the recursion for $n\leqslant 20$ and continued fraction approximants for $n>20$.

For the Druyvesteyn polynomials we only obtained the first two terms in the asymptotic expansions for α_n and β_n analytically. We attempted to calculate higher order terms

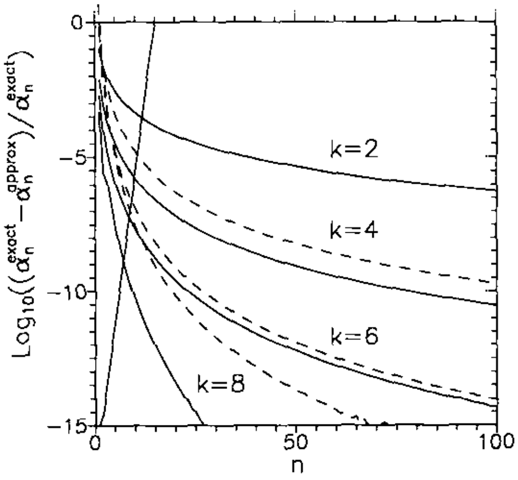

FIGURE 1

TABLE II

Asymptotic Series Coefficients b_k for the Bimode Polynomials with $a=b=2$

k	b_k
0	2.8867(−1)
1	1.6666(−1)
2	4.8112(−2)
3	0.0000(0)
4	8.0187(−3)
5	6.9444(−3)
6	−5.3458(−3)
7	−4.6296(−3)
8	−1.1415(−3)

in the asymptotic series numerically, but found that the two linear equations for a_2 and b_2 (see Section 3c) are linearly dependent. Table III gives the first two coefficients in the asymptotic expansions for α_n and β_n (with $a=1$). Figure 3 shows the logarithm of the relative error in α_n as a function of n and k.

As mentioned previously, the main objective is to generate recurrence coefficients and the corresponding quadrature weights and points for arbitrary weight function determined by a particular physical problem. The procedures developed in this paper to calculate the lower order coefficients in double precision and the remainder from the leading term in the asymptotic expansion appears to be promising. One aspect of this is the extent to which the approximate set of recurrence coefficients correspond to the original weight function. This involves what is referred to as the classical moment problem, that is, the determination of the weight function from a known set of moments or, equivalently, from the set of α_n and β_n coefficients. We have used the discrete Stieltjes procedure discussed by Langhoff [22] based on the earlier work of Shohat and Tamarkin

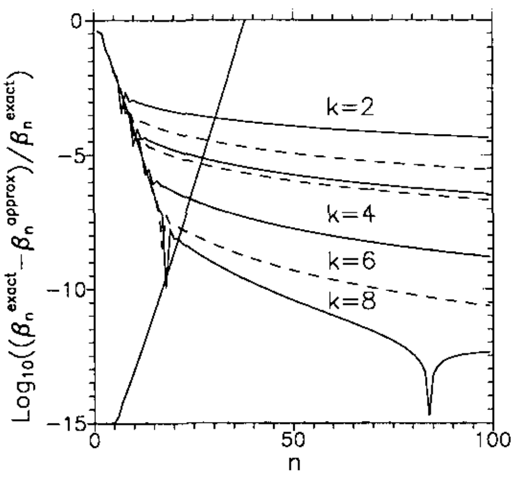

FIGURE 2

TABLE III

Asymptotic Series Coefficients a_k and b_k for the Druyvesteyn Polynomials with $a=1$

k	a_k	b_k
0	5.8143(−1)	8.4515(−2)
1	2.1803(−1)	4.2257(−2)

TABLE IV

Convergence of the Quadrature Points, x_i ($N=20$), versus the Order of the Asymptotic Expansion for $w(x)=x^2e^{-x^2}$

i	$k=0$	$k=1$	$k=2$	Exact	% diff[(a)]
1	0.02358	0.05436	0.06102	0.06027	1.243
2	0.13628	0.15614	0.16032	0.15984	0.301
3	0.27952	0.29642	0.29961	0.29928	0.111
4	0.44630	0.47126	0.47538	0.47489	0.101
5	0.65432	0.68015	0.68306	0.68271	0.052
6	0.89309	0.91655	0.91922	0.91891	0.034
7	1.14599	1.17755	1.18049	1.18011	0.032
8	1.42754	1.46181	1.46378	1.46350	0.019
9	1.73297	1.76533	1.76712	1.76687	0.014
10	2.04526	2.08709	2.08896	2.08867	0.014
11	2.38065	2.42723	2.42816	2.42795	0.009
12	2.73846	2.78379	2.78460	2.78441	0.007
13	3.09813	3.15799	3.15868	3.15845	0.007
14	3.48642	3.55185	3.55139	3.55125	0.004
15	3.89494	3.96546	3.96518	3.96503	0.004
16	4.30467	4.40536	4.40362	4.40350	0.003
17	4.77503	4.87502	4.87289	4.87283	0.001
18	5.20400	5.39030	5.38377	5.38384	−0.001
19	5.72095	5.96544	5.95805	5.95808	−0.001
20	6.42085	6.65932	6.65288	6.65291	−0.001

[(a)] % diff $=100\times(x_i^{\mathrm{exact}}-x_i^{(k=2)})/x_i^{\mathrm{exact}}$.

TABLE V

Convergence of the Quadrature Weights, w_i ($N=20$), versus Order of the Asymptotic Expansion for $w(x)=x^2e^{-x^2}$

i	$k=0$	$k=1$	$k=2$	Exact	% diff[(a)]
1	0.674748(−4)	0.230648(−3)	0.292216(−3)	0.284521(−3)	2.705
2	0.237173(−2)	0.292250(−2)	0.299696(−2)	0.299003(−2)	0.232
3	0.110842(−1)	0.126517(−1)	0.129921(−1)	0.129546(−1)	0.289
4	0.302334(−1)	0.342622(−1)	0.346840(−1)	0.346259(−1)	0.168
5	0.636592(−1)	0.651661(−1)	0.650890(−1)	0.651032(−1)	−0.022
6	0.881967(−1)	0.901870(−1)	0.904892(−1)	0.904512(−1)	0.042
7	0.933812(−1)	0.946743(−1)	0.943194(−1)	0.943464(−1)	−0.029
8	0.790182(−1)	0.742682(−1)	0.738123(−1)	0.738744(−1)	−0.084
9	0.460680(−1)	0.431515(−1)	0.430210(−1)	0.430399(−1)	−0.044
10	0.203998(−1)	0.185101(−1)	0.183674(−1)	0.183855(−1)	−0.099
11	0.687644(−2)	0.567438(−2)	0.563968(−2)	0.564628(−2)	−0.117
12	0.149018(−2)	0.121832(−2)	0.121479(−2)	0.121576(−2)	−0.080
13	0.239198(−3)	0.178668(−3)	0.177530(−3)	0.177774(−3)	−0.138
14	0.260954(−4)	0.168920(−4)	0.169172(−4)	0.169360(−4)	−0.111
15	0.156451(−5)	0.990858(−6)	0.993303(−6)	0.994232(−6)	−0.093
16	0.734920(−7)	0.329204(−7)	0.332192(−7)	0.332639(−7)	−0.134
17	0.129572(−8)	0.551796(−9)	0.564401(−9)	0.564529(−9)	−0.023
18	0.236851(−10)	0.381789(−11)	0.401897(−11)	0.402036(−11)	−0.035
19	0.428064(−13)	0.818611(−14)	0.840047(−14)	0.841300(−14)	−0.149
20	0.578266(−17)	0.213212(−17)	0.212607(−17)	0.212995(−17)	−0.182

[(a)] % diff $=100\times(w_i^{\mathrm{exact}}-w_i^{(k=2)})/w_i^{\mathrm{exact}}$.

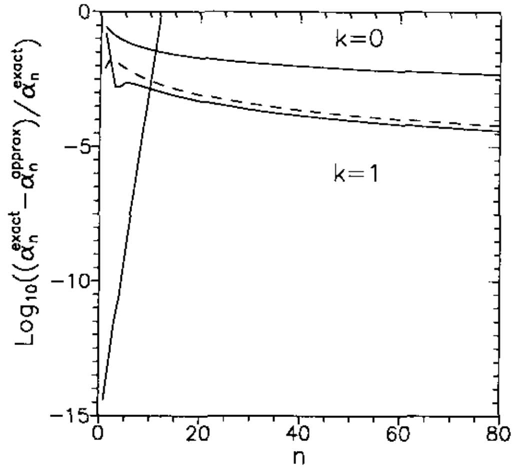

FIGURE 3

23] to generate the weight function from the approximate set of α_n and β_n coefficients. The approximate weight function is given by

$$w(\tilde{x}_i) = \frac{1}{2}\left[\frac{w_{i+1} + w_i}{x_{i+1} - x_i}\right], \tag{54}$$

where $\tilde{x}_i = \frac{1}{2}(x_{i+1} + x_i)$, and x_i and w_i are the points and weights corresponding to the approximate set of recurrence coefficients. A comparison of this approximate weight function and the exact speed weight function is shown in Fig. 4. The solid curve is the exact result, whereas the symbols were calculated with Eq. (54). This agreement is not unexpected since the lower order moments for the approximate and exact set of recurrence coefficients are essentially the same. Nevertheless, this demonstrates that the approximate procedures developed in this paper can be very useful.

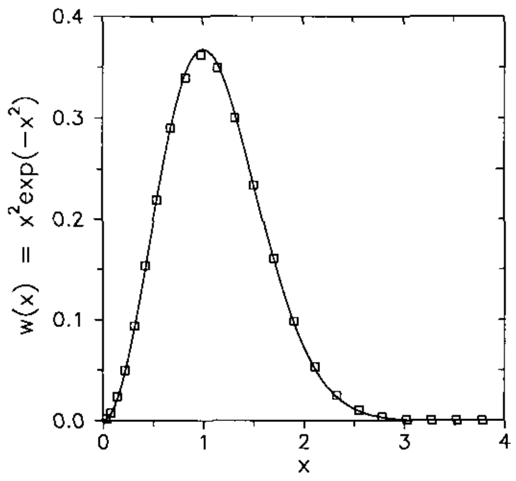

FIGURE 4

6. SUMMARY

In this paper we presented a derivation of the asymptotic expansion of the coefficients α_n and β_n in the three term recurrence relation for three sets of nonclassical orthogonal polynomials as defined by different weight functions and intervals: speed polynomials, bimode polynomials, and Druyvesteyn polynomials. In the case of *classical* orthogonal polynomials the recurrence relation coefficients α_n and β_n are simple functions of n. For these *nonclassical* polynomials, the coefficients α_n and β_n are determined by the solution of a set of nonlinear recurrence relations which are numerically unstable. Approximately one significant figure is lost in each iteration. However, the recurrence relations can be used together with multiple precision algorithms to calculate the recurrence coefficients up to $n = 100$ with 16 significant figures. This was done in previous papers for speed polynomials [10] and bimode polynomials [7], and for Druyvesteyn polynomials in the present paper.

For all three sets of polynomials, divergent asymptotic series expansions for the recurrence coefficients were derived and combined with continued fraction approximants to obtain accurate approximations for large n. The numerical values obtained in this way were compared with the exact values of α_n and β_n and the relative error evaluated. For the speed and bimode polynomials we were able to obtain an approximate set of α_n and β_n coefficients accurate to eight significant figures, using the recurrence relations in double precision for $n \leqslant 10$ and with the asymptotic expansions for $n > 10$. For the Druyvesteyn polynomials the first two terms in the asymptotic series approximant gave approximately 3-digit accuracy for $n > 10$. For all three sets of polynomials, the continued fraction approximants and asymptotic series expansions gave about the same accuracy. Greater than 8-digit accuracy requires that more terms in the asymptotic expansion be retained and that the series summation be performed using continued fractions or Padé approximants. However, if only 7-digit accuracy is required the asymptotic series expansion is sufficient.

The asymptotic series expansions for the coefficients α_n and β_n permitted a useful analysis of the numerical stability of the recurrence relations. This analysis shows that the recurrence relations are unstable for all n. Thus even using multiple precision airthmetic only allows one to calculate a finite number of α_n and β_n coefficients. This contrasts with the asymptotic approximations, where the accuracy *increases* with increasing n.

Shizgal [1, 7, 10] has shown that using nonclassical orthogonal polynomials as a basis set in the QDM technique often improves the convergence rate of the solution of differential and integral equations. The method introduced in the present paper presents a useful method for the accurate and efficient evaluation of the recurrence coefficients and corresponding quadrature points and weights.

This should find useful applications to the solution of differential and/or integral equations with the QDM, DVR, or similar spectral methods. In a future paper, we will use the Druyvesteyn polynomials in the solution Fokker–Planck-type equations for electron transport to investigate the accuracy of QDM in comparison with other numerical techniques.

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21. In the absence of exact values of the a_k and b_k we obtain an indirect measure of their accuracy by comparing the continued fraction approximants of order k with the multiple precision solutions α_n, β_n for all n. We find that beyond $k \simeq 10$ both the asymptotic series approximants and the continued fraction approximants diverge from the multiple precision solutions, presumably due to propagation of roundoff errors. The problem arises from the coefficients in the Taylor expansion of $(1+\varepsilon)^{-k}$ in the terms $\tilde{\alpha}_{n+1} = \sum_{k=0}^{\infty} a_k \varepsilon^k (1+\varepsilon)^{-k}$ and $\tilde{\beta}_{n+1} = \sum_{k=0}^{\infty} b_k \varepsilon^k (1+\varepsilon)^{-k}$ in Eqs. (32) and (33) which grow rapidly with increasing k and which alternate in sign.
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