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ABSTRACT

This paper presents the generalization of a semi-analytical technique for the evaluation of angular integrals appearing in the generation of elastic and discrete inelastic transfer matrices for transport codes. Whereas the generalized series expansions present a high degree of complexity, which puts them at a disadvantage in comparison with the Gaussian quadrature technique, the recursion relations developed in this study are superior to the quadrature formulas in those cases where the propagation of round-off errors is not significant.

1. INTRODUCTION

Among the techniques used at present in generating transfer matrices for elastic and discrete inelastic scattering in processing codes, the technique used in the NJOY [1,2] system is one of the most accurate and reliable, insofar as the numerical algorithm used [3] is concerned. This algorithm involves the evaluation of the angular integrals [4]

$$X_{k,\ell}(E',g) = \int_{\omega_g(E')}^{\omega_{g-1}(E')} d\omega \, P_k(\mu) \, P_\ell(\omega) \tag{1}$$

by means of the Gaussian quadrature formula. In equation (1), $P_n(x)$ denotes the Legendre polynomial of order n, ω is the cosine of the scattering angle in the centre-of-mass system and μ is the cosine of the scattering angle in the laboratory system, related to ω by [5]

$$\mu = \left[1 + \gamma(E')\omega\right] \left[1 + 2\gamma(E')\,\omega + \gamma^2(E')\right]^{-1/2} , \tag{2}$$

where $\gamma(E') \in [0,A]$ is a parameter depending on the initial energy of the neutron, defined by

$$\gamma(E') = A\left(1 + \frac{A+1}{A}\,\frac{Q_i}{E'}\right)^{1/2} \quad , \tag{3}$$

A being the ratio between the mass of the scattering nucleus and that of the neutron and $Q_i \leqslant 0$, $i = 0, 1, \ldots, I$, the excitation energy of the level i of the scattering nucleus, with the fictitious level $Q_0 = 0$ representing elastic scattering. Also in Eq. (1), g denotes the final energy group, with $E \in (E_g, E_{g-1})$, and the limits of integration are given by $\omega_g(E') = \max\{-1, \min[\omega(E_g,E'), 1]\}$ and $\omega_{g-1}(E') = \min\{1, \max[\omega(E_{g-1},E'), -1]\}$, where

$$\omega(E,E') = \frac{1}{2}\left\{\left[(A+1)^2\frac{E}{E'} - 1\right]\frac{1}{\gamma(E')} - \gamma(E')\right\} \quad . \tag{4}$$

The main difficulty encountered in evaluating $X_{k,\ell}(E',g)$ by numerical quadratures consists in the determination of the lower order of quadrature necessary for the result obtained to satisfy a given accuracy criterion for all the k's and ℓ's desired. Since the theoretical estimates of the errors associated with the quadratures are difficult to evaluate in this case, this determination has to be made numerically in actual practice. A numerical study [6], made for k = 0 and 1 and $\ell = 1, 2, \ldots, 20$, reached the conclusion that the lower order of quadrature for a pre-established accuracy criterion can vary appreciably with $\gamma(E')$ and the size of the integration interval $[\omega_g(E'), \omega_{g-1}(E')]$ - a fact which complicates the solution of this question.

For the cases of k = 0 and k = 1, which provide all the information necessary for generating transfer matrices for the scattering codes, a semi-analytical technique was developed which uses recursion relations and series expansions as alternatives to the numerical quadratures [4]. A comparison between the two techniques [6] warranted the conclusion that, for k = 0 and k = 1, the semi-analytical technique offers greater computational effectiveness. The generalization of the series expansions for the generation of transfer matrices for transport codes, in which it is often necessary to have $k > 1$, is obtained in this study; the resulting expressions present a high degree of complexity, which - from the computational point of view - puts them at a disadvantage compared to the Gaussian quadratures. By contrast, the generalization - as obtained in this study - of the recursion relations presented in Ref. [4] affords an effective and economic means of processing the evaluation of Eq. (1) within the limit $\gamma(E') \to 1$, which is extremely difficult for the technique of numerical quadratures and also for that of series expansions.

To simplify the notation, the dependence of $X_{k,\ell}(E',g)$ on E' and g continues to be implicit in the subsequent equations and the limits of integration in Eq. (1) will be denoted by $a = \omega_g(E')$ and $b = \omega_{g-1}(E')$.

2. EXPRESSIONS FOR $X_{k,\ell}$

Series expansions for $X_{k,\ell}$ can be derived by following a procedure similar to that proposed by Amster [7,8] for the transformation matrices of Zweifel and Hurwitz [9], which are a special case of the $X_{k,\ell}$ which are studied here. Such expansions make use of representations of μ in terms of the functions which are generatrices of Legendre polynomials like those used in Ref. [4], expansions of $P_k(\mu)$ in Taylor series and Clebsch-Gordon expansions for the product $P_m(\omega)\ P_\ell(\omega)$.

2.1. Case of $\gamma < 1$

In accordance with Amster [7], we can write

$$X_{k+1,\ell} = \left(\frac{2k+1}{k+1}\right)\int_a^b d\omega\ \mu P_k(\mu)\ P_\ell(\omega) - \left(\frac{k}{k+1}\right) X_{k-1,\ell} \quad , \tag{5}$$

which can, after use of the representation

$$\mu = (1 + \gamma\omega)\sum_{m=0}^{\infty}(-1)^m\ \gamma^m\ P_m(\omega), \tag{6}$$

for $\gamma < 1$, be rewritten as

$$X_{k+1,\ell} = \left(\frac{2k+1}{k+1}\right)\int_a^b d\omega\ P_k(\mu)\sum_{m=0}^{\infty}\gamma^m f_m(\gamma)\ P_m(\omega)P_\ell(\omega) - \left(\frac{k}{k+1}\right) X_{k-1,\ell} \quad , \tag{7}$$

where

$$f_m(\gamma) = (-1)^m\left[\left(\frac{m-1}{2m-1}\right) - \left(\frac{m+1}{2m+3}\right)\gamma^2\right] \quad . \tag{8}$$

The Clebsch-Gordon expansion

$$P_m(\omega)\ P_\ell(\omega) = \sum_{j=0}^{J_s} A_{j,\ell,m}\ P_{\ell+m-2j}(\omega) \quad , \tag{9}$$

where $J_s = \min(\ell, m)$ and the coefficients $A_{j,\ell,m}$ are given explicitly in Ref. [10], enables Eq. (7) to be reduced to

$$X_{k+1,\ell} = \left(\frac{2k+1}{k+1}\right) \sum_{m=0}^{\infty} \gamma^m f_m(\gamma) \sum_{j=0}^{J_s} A_{j,\ell,m} X_{k,\ell+m-2j} - \left(\frac{k}{k+1}\right) X_{k-1,\ell} \quad . \tag{10}$$

Equation (10) can be used recursively in k to calculate the $X_{k,\ell}$ of interest, from $X_{0,\ell}$ and $X_{1,\ell}$, which can be calculated as described in Ref. [4]. Once an accuracy criterion has been established, the series which appears in Eq. (10) can be truncated for m = M, in such a way that the relative contribution of the term of order γ^{M+1} is negligible. Note that, in order to evaluate $X_{k+1,\ell}$ for $\ell = 0, 1, \ldots, L$, it is necessary to have evaluated $X_{k,\ell}$, $\ell = 0, 1, \ldots, L+M$, in addition, of course, to $X_{k-1,\ell}$, $\ell = 0, 1, \ldots, L$. The low computational effectiveness of Eq. (10) then follows from the need to calculate a large number of superfluous $X_{k,\ell}$ elements in intermediate calculations.

2.2. Case of $\gamma > 1$

Despite the fact that the procedure for $\gamma < 1$ is also applicable in deriving a series expansion for $X_{k,\ell}$ valid for $\gamma > 1$, it is more convenient in this case to use a Taylor series expansion like the one employed by Amster [8] in studying the transformation matrices of Zweifel and Hurwitz.

Initially, it is readily verifiable [8] that

$$\left.\frac{\partial^m P_k(\mu)}{\partial \gamma^m}\right|_{\gamma=\infty} = m! \sum_{j=J_i}^{k+m} b^m_{k,j} \, P_j(\omega) \quad , \tag{11}$$

where $J_i = \max(k - m, 0)$ and the constants $b^m_{k,j}$ can be calculated recursively with

$$b^m_{k,j} = \frac{1}{m} \left[\frac{(j+1)\,(j+3-m)}{(2j+3)} \, b^{m-1}_{k,j+1} - \frac{j(j+m-2)}{(2j-1)} \, b^{m-1}_{k,j-1} \right] , \tag{12}$$

and the initial values $b^0_{k,j} = \delta_{kj}$. Thus, $P_k(\mu)$ can be expanded in Taylor series around $\gamma = \infty$ and the result substituted in Eq. (1), giving

$$X_{k,\ell} = \sum_{m=0}^{\infty} \gamma^{-m} \sum_{j=J_i}^{k+m} b^m_{k,j} \, S_{j,\ell} \quad , \tag{13}$$

where

$$S_{j,\ell} = \int_a^b d\omega \; P_j(\omega) \; P_\ell(\omega) \tag{14}$$

can be calculated with the expressions supplied in Ref. [4]. Note that as a result of the truncation of the series in $m = M$, the calculation of $X_{k,\ell}$ for $\ell = 0, 1, \ldots, L$, requires the evaluation of $S_{j,\ell}$, $j = J_i, J_i + 1, \ldots, k+M$ and $\ell = 0, 1, \ldots, L$. The existence of the double summation compromises the computational effectiveness of Eq. (13).

2.3. Case of $\gamma \to 1$

It is obvious that the number of terms to be considered in the series present in Eqs (10) and (13), for a given accuracy criterion, increases as γ approaches 1. It therefore becomes necessary to use an alternative procedure for $\gamma \to 1$. This procedure makes use of the recursion relations developed in Ref. [4] for generating the two first lines $X_{0,\ell}$ and $X_{1,\ell}$, $\ell \geqslant 0$. For completing the two columns $X_{k,0}$ and $X_{k,1}$, $k = 2, 3, \ldots, k$, we can use the following recursion relations, derived by applying the basic properties of the Legendre polynomials, as shown in the Appendix.

$$X_{2,0} = X_{0,0} + \frac{3}{8}\gamma \left[\omega^2 - \left(\gamma + \frac{1}{\gamma}\right)\omega + \frac{1}{2}\left(\gamma - \frac{1}{\gamma}\right)^2 \ln(1+2\gamma\omega+\gamma^2)\right]\Bigg|_{\omega=a}^{\omega=b}, \tag{15a}$$

$$X_{k+2,0} = \left(\frac{1}{2k-1}\right)\left[2(2k+1)\,X_{k,0} - (2k+3)\,X_{k-2,0}\right] + \left[\frac{(2k+1)(2k+3)}{k(k+1)}\right]\gamma\, X_{k,1}$$

$$-\left(\frac{1}{\gamma}\right)(1+2\gamma\omega+\gamma^2)\left\{\frac{1}{k}\left[P_{k+2}(\mu) - P_k(\mu)\right] + \left[\frac{2k+3}{(k+1)(2k-1)}\right]\left[P_k(\mu) - P_{k-2}(\mu)\right]\right\}\Bigg|_{\omega=a}^{\omega=b} \tag{15b}$$

and

$$X_{k+1,1} = \left(\frac{1}{k+5}\right)\left\{\left(\frac{1}{\gamma^2}\right)(1+\gamma\omega)(1+2\gamma\omega+\gamma^2)\left[P_{k+1}(\mu) - P_{k-1}(\mu)\right]\Bigg|_{\omega=a}^{\omega=b} - \left[(k+2)\gamma + \frac{3}{\gamma}\right]X_{k+1,0}\right.$$

$$\left. -(k-4)\,X_{k-1,1} - \left[(k-1)\gamma - \frac{3}{\gamma}\right]X_{k-1,0}\right\} . \tag{15c}$$

Initially, Eq. (15a) gives $X_{2,0}$; subsequently, Eq. (15b) with $K = 1$ gives $X_{3,0}$ and Eq. (15c) with $k = 1$ gives $X_{2,1}$. Continuing to use Eqs (15b) and (15c) alternately for $k = 2, 3, \ldots$, once the two first lines and columns

have been obtained, the remaining $X_{k,\ell}$ constituents can be calculated with the recursion relation derived in the manner shown in the Appendix,

$$X_{k+2,\ell+1} = -\left(\frac{\ell}{\ell+1}\right)X_{k+2,\ell-1} - \left(\frac{2\ell+1}{2\ell+2}\right)\left(\gamma + \frac{1}{\gamma}\right)X_{k+2,\ell} + \left(\frac{2k+1}{2\ell+2}\right)\left(\frac{\alpha_{\ell-1}}{\alpha_{k+1}}\right)\gamma X_{k,\ell-2}$$

$$+ \left(\frac{\ell}{\ell+1}\right)\left[1 + \frac{\alpha_{k-1}}{\alpha_{k+1}}\right]X_{k,\ell-1} - \left\{\left(\frac{2k+1}{2\ell+2}\right)\left(\frac{\alpha_{\ell+1}+\alpha_{\ell-1}}{\alpha_{k+1}}\right)\gamma - \left(\frac{2\ell+1}{2\ell+2}\right)\left[1 + \frac{\alpha_{k-1}}{\alpha_{k+1}}\right]\right.$$

$$\left.\times\left(\gamma + \frac{1}{\gamma}\right)\right\}X_{k,\ell} + \left[1 + \frac{\alpha_{k-1}}{\alpha_{k+1}}\right]X_{k,\ell+1} + \left(\frac{2k+1}{2\ell+2}\right)\left(\frac{\alpha_{\ell+1}}{\alpha_{k+1}}\right)\gamma X_{k,\ell+2} - \left(\frac{\alpha_{k-1}}{\alpha_{k+1}}\right)$$

$$\times\left[\left(\frac{\ell}{\ell+1}\right)X_{k-2,\ell-1} + \left(\frac{2\ell+1}{2\ell+2}\right)\left(\gamma + \frac{1}{\gamma}\right)X_{k-2,\ell} + X_{k-2,\ell+1}\right], \qquad (16)$$

making ℓ vary from 1 to L + K − (k + 3) for k varying from 0 to K−2. The quantity α_n present in Eq. (16) is given by $n(n + 1)/(2n + 1)$.

3. RESULTS

The recursive scheme presented in Section 2.3 was implemented in the CYBER 170/750 system of the IEAv and compared with the Gaussian quadrature technique. The comparisons performed took into consideration the calculation of $X_{k,\ell}$ for k = 0, 1, ..., 10 and ℓ = 0, 1, ..., 20 for different values of γ and of the integration limits a and b. Adopting the same accuracy criterion as that used in Ref. [6], by which the transfer matrices can be calculated with 5 significant algorithms, it was possible to determine numerically that the recursion scheme can be used with assurance for $2/3 \leq \gamma \leq 4/3$, without the propagation of round-off errors compromising its efficiency. This determination took into account limits greater than 10 and 20 in k and ℓ, respectively. If these limits are reduced, especially the limit in ℓ, the validity range of the recursive scheme can be extended. For example, in the case of elastic scattering in deuterium (γ = 1.997), there are no problems in using the recursive scheme since the upper limit in ℓ given in File 4 of ENDF/B is equal to 6.

Table 1 shows some values of $X_{k,\ell}$ calculated by the recursive scheme for elastic scattering in hydrogen (γ = 0.99917) with a = −1 and b = 0.9.

TABLE 1. – $X_{k,\ell}$ for $\gamma = 0.99917$, $a = -1$ and $b = 0.9$, calculated with the recursive scheme.

k	$\ell = 0$	$\ell = 1$	$\ell = 2$	$\ell = 3$	$\ell = 4$	$\ell = 5$	$\ell = 6$	$\ell = 7$	$\ell = 8$	$\ell = 9$	$\ell = 10$
0	1,900000	-0,095000	-0,085500	-0,072438	-0,057071	-0,040827	-0,025130	-0,011235	-0,000099	0,007713	0,012062
1	1,235699	0,172179	-0,122231	-0,059180	-0,062105	-0,037575	-0,026808	-0,010277	-0,001107	0,007859	0,011334
2	0,404999	0,408075	-0,082468	-0,070059	-0,055421	-0,039950	-0,024947	-0,011649	-0,000922	0,006650	0,010967
3	-0,092595	0,369804	0,072103	-0,095019	-0,043459	-0,044168	-0,021895	-0,013805	-0,000566	0,004837	0,010452
4	-0,171913	0,125706	0,215468	-0,064690	-0,051739	-0,037927	-0,024536	-0,012512	-0,002760	0,004325	0,008505
5	-0,082203	-0,078360	0,206638	0,044709	-0,070074	-0,028101	-0,028566	-0,010539	-0,005578	0,003830	0,006114
6	-0,043877	-0,116685	0,066425	0,148830	-0,046261	-0,034966	-0,023790	-0,013733	-0,005296	0,000955	0,005016
7	-0,068516	-0,065620	-0,059993	0,147294	0,038059	-0,049935	-0,016276	-0,018103	-0,004523	-0,002401	0,003945
8	-0,077005	-0,039173	-0,083861	0,049441	0,119492	-0,031128	-0,022800	-0,014959	-0,008300	-0,002937	0,000777
9	-0,052954	-0,050970	-0,047310	-0,042079	0,119947	0,036665	-0,036130	-0,009548	-0,013039	-0,003021	-0,002710
10	-0,035281	-0,054110	-0,026854	-0,059554	0,044280	0,102792	-0,021339	-0,016121	-0,011195	-0,007056	-0,003587

TABLE 2. – Comparison of $X_{k,20}$ for γ = 0.99917 and various integration intervals.

Interval	Method*/	k = 2	k = 3	k = 4	k = 5	k = 6	k = 7	k = 8	k = 9	k = 10
	Q(40)	-0,004274	-0,003957	-0,003661	-0,003306	-0,002766	-0,002172	-0,001700	-0,001214	-0,000545
[-1 ; 0,9]	Q(80)	-0,004273	-0,003966	-0,003663	-0,003295	-0,002762	-0,002185	-0,001704	-0,001200	-0,000539
	R	-0,004270	-0,003976	-0,003669	-0,003284	-0,002754	-0,002195	-0,001715	-0,001191	-0,000526
	Q(4)	0,004260	0,003989	0,003639	0,003218	0,002738	0,002210	0,001648	0,001065	0,000478
[0,9 ; 1]	Q(6)	0,004274	0,004006	0,003659	0,003243	0,002769	0,002248	0,001695	0,001124	0,000551
	R	0,004274	0,004006	0,003659	0,003243	0,002769	0,002248	0,001695	0,001124	0,000551
	Q(10)	0,003090	-0,000496	-0,001427	-0,000310	0,000928	0,000664	-0,001172	-0,003158	-0,003628
[-0,4;0,6]	Q(12)	0,003090	-0,000495	-0,001427	-0,000311	0,000926	0,000661	-0,001173	-0,003155	-0,003617
	R	0,003090	-0,000495	-0,001427	-0,000311	0,000926	0,000661	-0,001173	-0,003155	-0,003617

*/ Q(N): quadrature of order N

R: recursion

TABLE 3. - Comparison of $X_{k,5}$ for $\gamma = 1.997$ and various integration intervals.

Interval	Method*/	k = 2	k = 3	k = 4	k = 5	k = 6	k = 7	k = 8	k = 9	k = 10
	Q(20)	-0,061546	0,015582	-0,091891	-0,063107	0,051262	0,088679	0,053692	0,012208	-0,008523
[-1; 0,9]	Q(24)	-0,061546	0,015582	-0,091891	-0,063107	0,051262	0,088679	0,053691	0,012210	-0,008531
	R	-0,061546	0,015582	-0,091891	-0,063107	0,051262	0,088679	0,053691	0,012210	-0,008532
	Q(2)	0,039254	0,037728	0,035761	0,033406	0,030726	0,027791	0,024672	0,021441	0,018169
[0,9; 1]	Q(4)	0,039261	0,037741	0,035785	0,033450	0,030801	0,027914	0,024866	0,021738	0,018606
	R	0,039261	0,037741	0,035785	0,033450	0,030801	0,027914	0,024866	0,021738	0,018606
	Q(6)	0,048369	-0,003890	-0,059166	-0,052661	0,007377	0,051267	0,036672	-0,007133	-0,028197
[-0,4;0,6]	Q(8)	0,048369	-0,003890	-0,059166	-0,052662	0,007377	0,051269	0,036673	-0,007143	-0,028308
	R	0,048369	-0,003890	-0,059166	-0,052662	0,007377	0,051269	0,036673	-0,007143	-0,028308

*/ Q(N): quadrature of order N

R: recursion

TABLE 4. - Orders of Gauss-Legendre quadratures recommended for obtaining $X_{k,\ell}$, $k = 0.1,\ldots, 10$ and $\ell = 0.1,\ldots, 20$, within the accuracy criterion mentioned in the text*/.

Magnitude of the integration interval	$\gamma = 1/100$	$\gamma = 1/10$	$\gamma = 1/2$	$\gamma = 2/3$	$\gamma = 4/3$	$\gamma = 3/2$	$\gamma = 2$	$\gamma = 10$	$\gamma = 100$
0,1	6	6	8	10	16	12	10	8	8
0,2	8	8	10	16	20	16	12	10	10
0,3	8	8	12	16	24	20	16	10	10
0,4	8	10	16	20	32	20	16	12	12
0,5	10	10	16	20	32	24	20	16	12
0,6	10	10	16	24	32	24	20	16	16
0,7	10	10	20	24	40	32	20	16	16
0,8	10	12	20	24	40	32	24	16	16
0,9	10	12	20	32	40	32	24	16	16
1,0	12	12	20	32	40	40	24	16	16
1,1	12	12	24	32	80	40	32	16	16
1,2	12	12	24	32	80	40	32	20	16
1,3	12	12	24	32	80	40	32	20	16
1,4	12	12	24	32	80	40	32	20	16
1,5	12	16	24	40	80	40	32	20	16
1,6	12	16	24	40	80	40	32	20	20
1,7	12	16	24	40	80	80	32	20	20
1,8	12	16	32	40	80	80	32	20	20
1,9	12	16	32	40	80	80	40	20	20
2,0	12	16	32	40	80	80	40	20	20

*/ For $\gamma \in [2/3, 4/3]$ the recursive scheme should be used.

TABLE 5. – Approximate ratio of the time for carrying out the Gauss-Legendre quadrature technique (T_Q) and the recursive technique (T_R), for the calculation of $X_{k,\ell}$, k = 0.1,..., 10 and ℓ = 0.1,..., 20.

Order of quadrature	T_Q/T_R	Order of quadrature	T_Q/T_R
2	0,3	16	2,3
4	0,6	20	2,8
6	0,9	24	3,3
8	1,2	32	4,5
10	1,4	40	5,6
12	1,7	80	11,0

In Table 2, the values of $X_{k,20}$, k = 2, 3, ..., 10 for γ = 0.99917 and various integration intervals, are compared with results of the Gauss-Legendre quadrature. It may be noted that, for the larger interval considered, the quadrature of order 80 is insufficient since, for the smaller intervals, quadratures of low order yield good results. Table 3 presents a comparison of the values of $X_{k,5}$, k = 2, 3, ..., 10, for γ = 1.997 and various integration intervals; we can also observe the greater difficulty of the quadrature technique in the treatment of the larger integration interval considered. By way of guidance for using the Gauss-Legendre quadrature technique for $\gamma < 2/3$ and $\gamma > 4/3$, Table 4 presents the recommended orders of quadrature for obtaining $X_{k,\ell}$, k = 0, 1, ..., 10 and ℓ = 0, 1, ..., 20 within the above-mentioned accuracy limits. For values of γ and integration magnitudes different from those shown in Table 4, use should be made of the larger order of quadrature shown by the values of γ and the integration magnitudes close to those desired. In the preparation of Table 4, it was observed that integration intervals containing or approximating the point -1 require higher orders of quadrature than intervals of equal magnitude further away from point -1, mainly for values of γ close to 1. The reason for this behaviour is that μ, in accordance with Eq. (2), is singular for $\omega = -(\gamma + 1/\gamma)/2$, and that a -1 tends to the left as $\gamma \to 1$. For $\gamma = 1$, the singularity of μ in -1 is removable. However, the values of Table 4 are rather conservative for integration intervals further

away from -1. Lastly, Table 5 shows the ratio of the time for carrying out the Gauss-Legendre quadrature technique to that for the recursive technique in the CYBER 170/750 system, which enables us to evaluate the computational advantage of the latter.

4. CONCLUSIONS

The recursive technique presented in this study is an accurate and effective method for calculating the angular integrals $X_{k,\ell}$ within the limits of $\gamma \to 1$. The technique can be used for $2/3 \leq \gamma \leq 4/3$, without the propagation of round-off errors prejudicing its use. For values of γ outside this interval, the technique of Gauss-Legendre quadratures is recommended, in accordance with the directions presented in Table 4 of this study.

APPENDIX

Derivation of the recursion relationships

To demonstrate Eq. (15b), the integration of

$$X_{k,1} = \int_a^b d\omega \; P_k(\mu)\, \omega \tag{A-1}$$

by parts gives

$$X_{k,1} = \frac{1}{2}\,(\omega^2-1)\,P_k(\mu)\,\Big|_a^b - \frac{1}{2}\int_a^b d\omega\,(\omega^2-1)\,P_k'(\mu)\,\frac{\partial\mu}{\partial\omega}\;, \tag{A-2}$$

which, with the use of the identity

$$\gamma^2(\omega^2-1) = (\mu^2-1)\,(1+2\gamma\omega+\gamma^2)\;, \tag{A-3}$$

and the properties

$$(2n+1)(x^2-1)\,P_n'(x) = n(n+1)\,[P_{n+1}(x) - P_{n-1}(x)] \tag{A-4a}$$

and

$$(2n+1)P_n(x) = P_{n+1}'(x) - P_{n-1}'(x)\;, \tag{A-4b}$$

followed by further integration by parts, may be rewritten as

$$X_{k,1} = \frac{1}{2}(\omega^2-1)\,P_k(\mu)\,\Big|_a^b + \frac{1}{2\gamma^2}\,\frac{k(k+1)}{2k+1}\,(1+2\gamma\omega+\gamma^2)\left\{\frac{1}{2k-1}\left[P_k(\mu) - P_{k-2}(\mu)\right]\right.$$

$$\left.-\frac{1}{2k+3}\left[P_{k+2}(\mu) - P_k(\mu)\right]\right\}\Big|_a^b - \frac{1}{\gamma}\,\frac{k(k+1)}{2k+1}\left\{\frac{1}{2k-1}\left[X_{k,0} - X_{k-2,0}\right]\right.$$

$$\left.-\frac{1}{2k+3}\left[X_{k+2,0} - X_{k,0}\right]\right\}. \tag{A-5}$$

with the use of the identity (A-3) and the property

$$(2n+1)\,x\,P_n(x) = (n+1)\,P_{n+1}(x) + n\,P_{n-1}(x)\;, \tag{A-6}$$

the first term of the right-hand side of Eq. (A-5) can be combined with the second term and the result rearranged, giving Eq. (15b). As this

equation cannot be used for K = 0, the term $X_{2,0}$ is calculated explicitly, on the basis of

$$X_{2,0} = \int_a^b d\omega \; P_2(\mu) = \frac{1}{2} \int_a^b d\omega \left[3 \left(\frac{1+2\gamma\omega + \gamma^2 \omega^2}{1+2\gamma\omega + \gamma^2} \right) - 1 \right] , \tag{A-7}$$

which, after it is integrated, gives Eq. (15a).

To demonstrate Eq. (15c), the relation

$$(k+1) \left[X_{k+1,1} + \gamma X_{k+1,0} \right] + k \left[X_{k-1,1} + \gamma X_{k-1,0} \right] = (2k+1) \int_a^b d\omega (\omega+\gamma) \mu \; P_k(\mu) , \tag{A-8}$$

with the use of the identity

$$\gamma^2 (\omega+\gamma) \mu = (1 + \gamma\omega)(1 + 2\gamma\omega + \gamma^2) \frac{\partial \mu}{\partial \omega} , \tag{A-9}$$

and to the property (A-4b), followed by integration by parts, gives the desired result.

The general recursion relationship, expressed by Eq. (16), can be derived by using the relationship

$$\left[\frac{\ell(\ell+1)}{2\ell+1} \right] \left[X_{k,\ell+1} - X_{k,\ell-1} \right] = \left(\frac{1}{\gamma^2} \right) \int_a^b d\omega \, (1 + 2\gamma\omega + \gamma^2)(\mu^2 - 1) \, P_k(\mu) \, P'_\ell(\omega) \tag{A-10}$$

initally with ℓ replaced by $\ell + 1$, and later with ℓ replaced by $\ell - 1$, subtracting the two results and using the properties (A-4) and (A-6).

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