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ABSTRACT

A study is made of the computational efficiency of a semi-analytical technique which has recently been proposed for the evaluation of angular integrals encountered in the generation of the isotropic and linearly anisotropic components of transfer matrices for elastic and discrete inelastic scattering. From a comparison with the results obtained with the use of numerical quadratures it is concluded that the technique has computational advantages which recommend its implementation.

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1. INTRODUCTION

A semi-analytical technique has recently [1] been proposed for the evaluation of angular integrals encountered in the generation of the isotropic and linearly anisotropic components of transfer matrices for elastic and discrete inelastic scattering. The components of the expansion of the collision cross-section for transfer from group g' to group g in Legendre polynomials were expressed by

$$\sigma_x(g' \to g, k) = W_{g'}^{-1} \int_{E^*_{g'}}^{E^*_{g'-1}} dE'\, W(E')\, \sigma_x(E')\, F_k(E', g) \quad , \qquad (1)$$

where

$$F_k(E',g) = \frac{1}{2} \sum_{\ell=0}^{L} (2\ell+1)\, f_x(\dot{E}',\ell)\, X_{k,\ell}(E',g) \quad , \tag{2}$$

and the remaining quantities were defined earlier [1]. In Eq. (2) functions $X_{k,\ell}(E',g)$ represent the angular integrals [1]

$$X_{k,\ell}(E',g) = \int_{\omega_g(E')}^{\omega_{g-1}(E')} d\omega\, P_k \left\{ [1+\gamma(E')\omega][1+2\gamma(E')\omega+\gamma^2(E')]^{-1/2} \right\} P_\ell(\omega) \tag{3}$$

which are the subject of this study. Since generally in neutron calculations only the isotropic (k = 0) and linearly anisotropic (k = 1) components are important, Ref. [1] was confined to the study of $X_{o,\ell}(E',g)$ and $X_{1,\ell}(E',g)$. Functions $X_{o,\ell}(E',g)$ were expressed by

$$X_{o,\ell}(E',g) = \left(\frac{1}{2\ell+1}\right) \left[P_{\ell+1}(\omega) - P_{\ell-1}(\omega) \right] \Big|_{\omega_g(E')}^{\omega_{g-1}(E')} \tag{4}$$

and functions $X_{1,\ell}(E',g)$ by

$$X_{1,\ell}(E',g) = Y_\ell(E',g) + \frac{\gamma(E')}{2\ell+1} \left[(\ell+1)\, Y_{\ell+1}(E',g) + \ell\, Y_{\ell-1}(E',g) \right] \tag{5}$$

where $Y_\ell(E',g)$ obey the recurrence relation for $\ell \geq 0$

$$(2\ell+3)Y_{\ell+1}(E',g) = (1-\delta_{o,\ell})(1-2\ell)Y_{\ell-1}(E',g) - (2\ell+1)\left[\frac{1}{\gamma(E')}+\gamma(E')\right] \tag{6}$$

$$\times \quad Y_\ell(E',g) + \frac{1}{\gamma(E')} \left\{ [1+2\gamma(E')\,\omega+\gamma^2(E')]^{1/2} \right.$$

$$\times \quad \left. \left[P_{\ell+1}(\omega) - P_{\ell-1}(\omega) \right] \right\} \Big|_{\omega_g(E')}^{\omega_{g-1}(E')}$$

Since the recurrence relation expressed by Eq. (6) becomes unstable for $\gamma(E') >> 1$ or $\gamma(E') << 1$, the following series representations were developed in Ref. [1]

$$X_{1,\ell}(E',g) = \sum_{m=0}^{\infty} (-1)^m S_{m,\ell}(E',g) \left[\left(\frac{m+2}{2m+3}\right) - \left(\frac{m}{2m-1}\right)\gamma^2(E') \right] \times \left[\frac{1}{\gamma(E')}\right]^{m+1}, \gamma(E') > 1 \quad , \tag{7}$$

and

$$X_{1,\ell}(E',g) = \sum_{m=0}^{\infty} (-1)^m S_{m,\ell}(E',g) \left[\left(\frac{m-1}{2m-1}\right) - \left(\frac{m+1}{2m+3}\right)\gamma^2(E') \right] \gamma^m(E') \quad , \gamma(E') < 1 \quad , \tag{8}$$

for alternative use in the recursive scheme formed by Eqs (5) and (6), when necessary. The purpose of the present study is to evaluate the computational efficiency of the technique of calculation of $X_{o,\ell}(E',g)$ and $X_{1,\ell}(E',g)$ summarized by Eqs (4)-(8) and to compare it with the technique which uses a representation of Eq. (3) in quadratures like that used in the NJOY system [2].

2. RESULTS

It is known that any comparison between execution times for different techniques is valid only when the techniques are used in such a way as would yield results with the same numerical accuracy. Thus, in this study the accuracy criterion imposed on $X_{o,\ell}(E',g)$ and $X_{1,\ell}(E',g)$, $\ell = 0, 1, \ldots, 20$, was so chosen as to guarantee a minimum of five correct significant digits in $F_k(E',g)$, $k = 0$ and 1, for both the techniques studied. With this criterion it was possible to determine, on numerical bases, that the recursive scheme of Eqs (5) and (6) can be used only for $2/5 \leq \gamma(E') \leq 5/2$. In this way, for $\gamma(E') > 5/2$ and $\gamma(E') < 2/5$ the present study used the series representations given in Eqs (7) and (8), respectively, truncated so as to provide the desired accuracy. For the calculation the quadratures of Eq (3) were used to test different orders of the Gauss-Legendre quadrature [3] and the lowest order in each case was chosen so as to guarantee the desired accuracy.

Table 1 compares the results obtained for $X_{1,\ell}(E',g)$ with $\gamma(E') = 1$, $\omega_g(E') = -1$ and $\omega_{g-1}(E') = 0.9$ by Eqs (5) and (6) and the results provided by Gauss-Legendre quadratures of order 20 and 40. The lowest order of quadrature found which would obey the pre-established criterion of accuracy was 32 in this case. Table 2 presents results similar to those in Table 1 for the case $\gamma(E') = 1$, $\omega_g(E') = 0.9$ and $\omega_{g-1}(E') = 1$. It will be noted that much lower orders of quadrature were sufficient. The lowest order required to guarantee the pre-established accuracy was 6 in this case.

Table 3 summarizes the approximate execution times in the CYBER 170/750 system of the Institute of Advanced Studies (IEAv) for the calculation of $X_{o,\ell}(E',g)$ and $X_{1,\ell}(E',g)$, $\ell = 0, 1, \ldots, 20$, obeying the stipulated accuracy criterion for various values of $\gamma(E')$ by the technique given in Ref. [1]. It was verified that the execution time was essentially independent of the $\omega_g(E')$ and $\omega_{g-1}(E')$ values considered; the values given in Table 3 can therefore be taken as representative values for any $\omega_g(E')$ and $\omega_{g-1}(E')$. This is not so when quadratures are used, as is shown in Table 4. Analysis of the results presented in Table 4 shows that the order of quadrature needed to guarantee the stipulated accuracy increases with increase in the size of the integration interval $[\omega_g(E'), \omega_{g-1}(E')]$. In the case of integration intervals of a size close to the maximum possible, i.e. 2, it is also noted that for $\gamma(E')$ equal or close to 1, the necessary orders of quadrature are sufficiently high.

From a comparison of the results given in Tables 3 and 4 it can be concluded that the recursive scheme of Eqs (5) and (6) is much more efficient in computational terms than the quadrature technique. Such a scheme can therefore be used with advantage in the generation of elastic transfer matrices for hydrogen and deuterium and also in a large part of the double-energy region for discrete inelastic scattering [4]. As for the series representations given by Eqs (7) and (8), they also in general offer a certain advantage in computational terms. This advantage tends to disappear when the integration interval is small. In the case of elastic scattering in heavy elements, the integration intervals tend to be large provided the group structure is not excessively fine; in this case, therefore, the use of Eq. (7) can reduce the time of execution to approximately half of the time required by the quadrature technique.

3. FINAL CONSIDERATIONS

Considering the computational advantages mentioned in the preceding section, the semi-analytical technique of angular integration proposed in Ref. [1] should serve as a useful tool for the generation of the isotropic and linearly anisotropic components of transfer matrices for elastic and discrete inelastic scattering. Additional tests will be carried out after implementation of the above technique with a view to a better evaluation of its performance in practice. It is also intended to study its possible generalization for the generation of components of transfer matrices for elastic and discrete inelastic scattering of a higher order.

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Table 1: Comparison of functions $X_{1,\ell}(E',g)$ calculated by the technique described in Ref. [1] with the results of the Gauss-Legendre quadrature for $\gamma(E') = 1$, $\omega_g(E') = -1$ and $\omega_{g-1}(E') = 0.9$.

ℓ	Ref [1]	Order of the Gauss-Legendre quadrature 20	40
0	1,23459	1,23462	1,23460
1	0,17284	0,17282	0,17284
2	-0,12258	-0,12256	-0,12257
3	-0,05894	-0,05896	-0,05894
4	-0,06229	-0,06227	-0,06229
5	-0,03742	-0,03745	-0,03743
6	-0,02694	-0,02691	-0,02693
7	-0,01017	-0,01019	-0,01017
8	-0,00120	-0,00118	-0,00120
9	0,00795	0,00792	0,00794
10	0,01125	0,01128	0,01126
11	0,01321	0,01319	0,01321
12	0,01125	0,01128	0,01126
13	0,00858	0,00855	0,00858
14	0,00419	0,00422	0,00419
15	0,00044	0,00040	0,00043
16	-0,00320	-0,00317	-0,00320
17	-0,00526	-0,00530	-0,00526
18	-0,00634	-0,00630	-0,00634
19	-0,00581	-0,00586	-0,00581
20	-0,00452	-0,00446	-0,00451

Table 2: Comparison of functions $X_{1,\ell}(E',g)$ calculated by the technique described in Ref. [1] with the results of the Gauss-Legendre quadrature for $\gamma(E') = 1$, $\omega_g(E') = 0.9$ and $\omega_{g-1}(E') = 1$.

ℓ	Ref. [1]	Order of the Gauss-Legendre quadrature 4	6
0	0,0987394	0,0987394	0,0987394
1	0,0938235	0,0938235	0,0938235
2	0,0844823	0,0844823	0,0844823
3	0,0716356	0,0716356	0,0716356
4	0,0565185	0,0565185	0,0565185
5	0,0405310	0,0405310	0,0405310
6	0,0250708	0,0250708	0,0250708
7	0,0113732	0,0113732	0,0113732
8	0,0003785	0,0003785	0,0003785
9	-0,0073561	-0,0073561	-0,0073561
10	-0,0116912	-0,0116912	-0,0116912
11	-0,0128829	-0,0128829	-0,0128829
12	-0,0115116	-0,0115116	-0,0115116
13	-0,0083739	-0,0083739	-0,0083739
14	-0,0043549	-0,0043550	-0,0043549
15	-0,0003006	-0,0003008	-0,0003006
16	0,0030913	0,0030908	0,0030913
17	0,0053490	0,0053477	0,0053490
18	0,0062627	0,0062597	0,0062627
19	0,0058790	0,0058725	0,0058790
20	0,0044570	0,0044438	0,0044570

Table 3: Approximate execution times for the calculation of $X_{o,\ell}(E',g)$ and $X_{1,\ell}(E',g)$, $\ell = 0, 1, \ldots, 20$, for different values of $\gamma(E')$ by the technique described in Ref. [1].

$\gamma(E')$	Time (ms)	Method	Terms in the series
0,01	4,8	Series	6
0,1	5,5	"	10
0,3	6,6	"	16
1	1,2	Recurrence	-
3	6,7	Series	17
10	5,5	"	10
100	4,8	"	6
235	4,6	"	5

Table 4: Approximate execution times and orders of the Gauss-Legendre quadrature used in the calculation of $X_{o,\ell}(E',g)$ and $X_{1,\ell}(E',g)$, $\ell = 0, 1, \ldots, 20$, for various intervals of integration $I = [\omega_g(E'); \omega_{g-1}(E')]$

γ (E')	I = [-1; 0,9]		I = [0,9 ; 1]		I = [-0,4;0,6]	
	Time (ms)	Order	Time (ms)	Order	Time (ms)	Order
0,01	9,7	12	5,0	6	8,3	10
0,1	12,9	16	5,0	6	9,7	12
0,3	12,9	16	5,0	6	9,7	12
1	25,9	32	5,0	6	9,7	12
3	12,9	16	5,0	6	9,7	12
10	12,9	16	5,0	6	9,7	12
100	9,7	12	5,0	6	8,3	10
235	9,7	12	5,0	6	8,3	10