NUREG/CR-0295
ORNL/NUREG/CSD-8

A METHOD OF GENERATING MULTIGROUP TRANSFER MATRICES USING AN ANALYTIC ANGULAR INTEGRATION FREE OF TRUNCATION ERROR

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Prepared for
U.S. Nuclear Regulatory Commission

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Manuscript Completed: August 1978
Date Published: September 1978

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Office of Nuclear Material Safety and Safeguards
U.S. Nuclear Regulatory Commission
Under FIN No. B0009

TABLE OF CONTENTS

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ABSTRACT

The evaluation of generalized multigroup transfer matrices for transport calculations requires a double integration extending over the primary and secondary energy groups where, for a given initial energy, the integration over the secondary energy group may be replaced by an integral over the possible scattering angles. The XLACS cross-section processing code presently used in the AMPX system treats this angular integral in an approximate manner. The more recent MINX cross-section processing code treats this angular integral analytically but can admit some small truncation error. These treatments are reviewed along with their weaknesses. In the present work, analytic expressions for these angular integrals are derived which are free of truncation error. Straightforward extensions to include inelastic and/or anisotropic scattering are included. FORTRAN routines are provided for nuclides having isotropic elastic scattering in the center-of-mass system.

A. Introduction

Many detailed multigroup transport calculations require group-to-group Legendre transfer coefficients to represent the scattering processes in various nuclides. These (fine group) constants must first be generated from the basic data. This report details an alternate technique for generating such data, given the total scattering cross section of a particular nuclide on a point-wise energy basis, $\sigma(E')$, and some information regarding the angular scattering distribution for each initial energy point.

Given the Legendre coefficients of the scattering cross section on a point-wise energy basis, $\sigma_\ell(\underline{r},E'\rightarrow E)$, the group-to-group Legendre transfer coefficients are defined as:

$$\sigma_\ell(\underline{r},g'\to g) \equiv \frac{\displaystyle\int_{E^g}^{E^{g-1}} \int_{E^{g'}}^{E^{g'-1}} \phi_\ell(\underline{r},E')\ \sigma_\ell(\underline{r},E'\to E)\ dE'\ dE}{\displaystyle\int_{E^{g'}}^{E^{g'-1}} \phi_\ell(\underline{r},E')\ dE'} \qquad (1)$$

where $\phi_\ell(\underline{r},E')$ are the Legendre coefficients of the angular flux distribution at each point. The use of these higher order angular flux coefficients as energy dependent weight functions has been shown to be necessary if the group-to-group Legendre transfer coefficients are to be consistent with their use in the solution of the Boltzmann transport equation by the spherical harmonics method[1]. Prior to performing a detailed transport calculation for the given configuration, such detailed information is not known. In practice, the higher order terms, $\phi_\ell(\underline{r},E')$, are replaced by an energy dependent weight function $\phi(E')$ whose form largely depends on the end use of the cross sections being generated. For the generation of cross sections which are problem independent, $\phi(E')$ may be $1/E'$ or some other assumed form. For the generation of cross sections which are mixture dependent, $\phi(E')$ may be the scalar flux resulting from the solution of the integral slowing down equation on a point-wise energy basis. In that event, the group-to-group Legendre transfer coefficients and the weight function, $\phi(E')$, may be developed in parallel, with a single point-wise sweep through the slowing down region. In either case, the group-to-group Legendre transfer coefficients are approximated as:

$$\sigma_\ell(g'\to g) = (1/\phi^{g'}) \int_{E^{g'}}^{E^{g'-1}} \phi(E') \left[\int_{E^g}^{E^{g-1}} \sigma_\ell(E'\to E)\ dE \right] dE' , \qquad (2)$$

where the spatial dependence of $\sigma_\ell(g' \to g)$ and $\sigma_\ell(E' \to E)$ is understood.

The Legendre coefficients, $\sigma_\ell(E' \to E)$, of the angular scattering cross section, $\sigma(E' \to E, \mu_L)$, are defined as:

$$\sigma_\ell(E' \to E) \equiv 2\pi \int_{-1}^{+1} \sigma(E' \to E, \mu_L)\ P_\ell(\mu_L)\ d\mu_L \ . \tag{3}$$

However, the angular scattering cross section, $\sigma(E' \to E, \mu_L)$ is of the form:

$$\sigma(E' \to E, \mu_L) = \frac{1}{2\pi}\ \sigma(E' \to E)\ \delta[\mu_L - \mu_L^*(E', E, Q, A)] \tag{4}$$

where, if μ_L represents the cosine of the angle of scatter in the lab system, $\mu_L^*(E', E, Q, A)$ represents the only possible value of that variable given the initial neutron energy (E'), the final neutron energy (E), the excitation energy (Q), and the atomic mass of the target nuclide (A). For two-body interactions, $\mu_L^*(E', E, Q, A)$ is given by:

$$\mu_L^*(E', E, Q, A) = \frac{1}{2}\left[(A+1)\sqrt{\frac{E}{E'}} - (A-1)\sqrt{\frac{E'}{E}} + \frac{AQ}{\sqrt{E'E}}\right] \tag{5}$$

which, when inserted into the definition of $\sigma_\ell(E' \to E, \mu_L)$ and $\sigma_\ell(E' \to E)$ yields:

$$\sigma_\ell(E' \to E) = \sigma(E' \to E)\ P_\ell[\mu_L(E', E, Q, A)] \ . \tag{6}$$

Integration of this quantity over the primary and secondary energy groups as noted in Eq. (2) then yields:

$$\sigma_\ell(g' \to g) = (1/\phi^{g'}) \int_{E^{g'}}^{E^{g'-1}} \phi(E') \left[\int_{E^g}^{E^{g-1}} P_\ell[\mu_L(E', E, Q, A)]\ \sigma(E' \to E)\ dE\right] dE' \ . \tag{7}$$

The accurate evaluation of this expression represents a severe computational burden which must be addressed by any cross-section processing code. The present method differs from previous approaches in that it yields an analytic solution for the integral on dE which is free of truncation error when the scattering function is given by a Legendre expansion in either the center-of-mass (C) or the lab (L) system.

B. Basic Theory

The scattering function, $\sigma(E'\rightarrow E)$, represents a distribution over the secondary energy (E) and hence over the scattering angle. If μ_c is the cosine of the scattering angle in the center-of-mass system, then those neutrons which scatter into dE about E must be the same ones which scatter into some $d\mu_c$ about μ_c such that:

$$\sigma(E'\rightarrow E)\, dE = \sigma(E')\, f(E',\mu_c)\, 2\pi d\mu_c \ , \tag{8}$$

where $\sigma(E')$ is the total scattering cross section for the particular nuclide at energy E', and $f(E',\mu_c)$ is the probability per unit solid angle that an incident neutron of energy E' scatters into an energy E associated with the scattering angle cosine μ_c in the center-of-mass system. This scattering probability function may, of course, be expanded as:

$$f(E',\mu_c) = \sum_{k=0}^{\infty} \frac{2k+1}{4\pi} f_k(E')\, P_k(\mu_c) \ . \tag{9}$$

The motivation for expanding this probability distribution function in the C system stems from the fact that scattering processes always appear more isotropic in the C system than in the L system. Hence, a good

representation of the scattering processes can be achieved with fewer terms in the C system. Indeed, most scattering involving the formation of a compound nucleus is isotropic in the C system, in which case the present expansion requires only one term in the C system. An infinite number of terms would be required to represent this same process exactly in the L system and even a moderately good representation for hydrogen would require a large number of terms. (Note, however, that the coefficients $\sigma_\ell(g' \to g)$ which will be calculated are in the L system, as necessary for subsequent transport calculations.)

For isotropic scattering in the C system,

$$f(E', \mu_c) = \frac{1}{4\pi} \tag{10}$$

and Eq. (8) becomes:

$$\sigma(E' \to E)\, dE = \frac{1}{2}\, \sigma(E')\, d\mu_c \ . \tag{11}$$

Hence, the integral on dE may be written as an integral on $d\mu_c$:

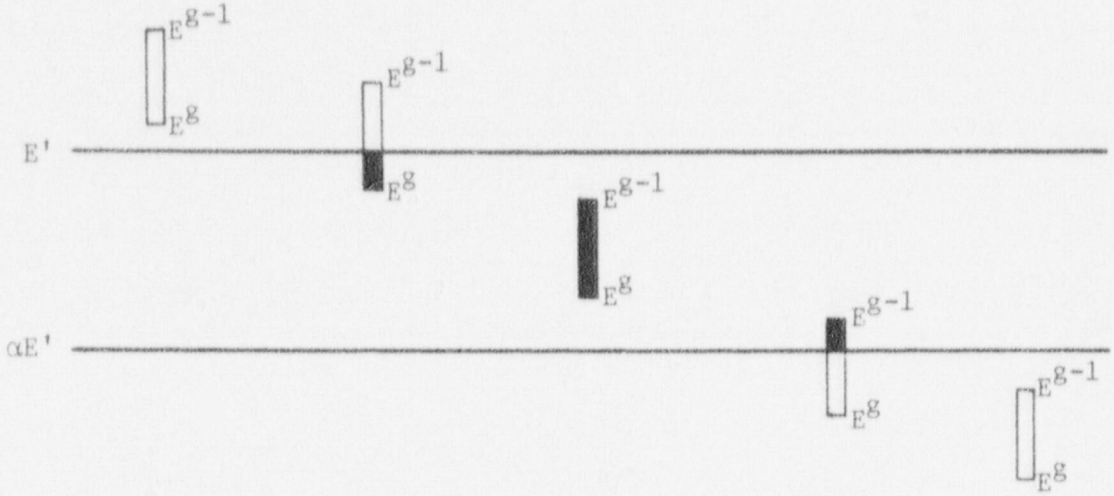
$$\int_{E^g}^{E^{g-1}} P_\ell[\mu_L(E', E, Q, A)]\, \sigma(E' \to E)\, dE =$$

$$= \frac{1}{2}\, \sigma(E') \int_{\mu_c(E', E_L, Q, A)}^{\mu_c(E', E_U, Q, A)} P_\ell[\mu_L(E', E(\mu_c), Q, A)]\, d\mu_c \tag{12}$$

where, if the scattering is also elastic in the C system (Q=0),

$$\mu_c = \gamma \mu_L^2 - \gamma + \mu_L(\gamma^2 \mu_L^2 + 1 - \gamma^2)^{1/2} \ , \quad \gamma = 1/A \ . \tag{13}$$

For neutron moderation due to elastic scattering in the C system, the secondary energy E must lie in the range $\alpha E' \leq E \leq E'$ where $\alpha = ((A-1)/(A+1))^2$.



$E_U=0$	$E_U=E'$	$E_U=E^{g-1}$	$E_U=E^{g-1}$	$E_U=0$
$E_L=0$	$E_L=E^g$	$E_L=E^g$	$E_L=\alpha E'$	$E_L=0$

Figure 1. Possible Location of an Arbitrary Secondary Energy Group Relative to the Range of Possible Secondary Energies E'→αE' and the Limits of Integration that Should be Used in Each Case.

An arbitrary secondary group having limits $E^{g-1} \rightarrow E^{g}$ may lie totally within, partially within, or totally outside the range $E' \rightarrow \alpha E'$ as shown in Fig. 1. The use of E_U and E_L as defined in Fig. 1 assures that E (and/or μ_c) will be integrated over the proper range for the given initial energy E'. The restriction to the range $E_U \rightarrow E_L$ would be necessary even had the change of variables not been made.

$P_\ell[\mu_L(E',E,Q,A)]$ is a simple polynomial in μ_L but the variable of integration is μ_c. Changing the variable of integration to μ_L will allow the integration to be done analytically in closed form. To do this, note that Eq. (13) can be differentiated to yield:

$$\frac{d\mu_c}{d\mu_L} = \gamma \left\{ 2\mu_L + \sqrt{\left(\frac{1-\gamma^2}{\gamma^2}\right) + \mu_L^2} + \frac{\mu_L^2}{\sqrt{\left(\frac{1-\gamma^2}{\gamma^2}\right) + \mu_L^2}} \right\} . \tag{14}$$

For $\gamma \leq 1$, Eq. (12) may now be written as:

$$\int_{E^g}^{E^{g-1}} P_\ell[\mu_L(E',E,Q,A)]\, \sigma(E' \rightarrow E)\, dE =$$

$$= \frac{1}{2}\, \sigma(E') \int_{\mu_c(E',E_L,Q,A)}^{\mu_c(E',E_U,Q,A)} P_\ell[\mu_L(E',E(\mu_c),Q,A)]\, d\mu_c \tag{15a}$$

$$= \frac{1}{2}\, \sigma(E') \int_{\mu_L(E',E_L,Q,A)}^{\mu_L(E',E_U,Q,A)} P_\ell[\mu_L(E',E,Q,A)] \left|\frac{d\mu_c}{d\mu_L}\right| d\mu_L \tag{15b}$$

$$= \frac{\gamma}{2}\, \sigma(E') \int_{\mu_L(E',E_L,Q,A)}^{\mu_L(E',E_U,Q,A)} \left\{ 2\mu_L + \sqrt{a^2+\mu_L^2} + \frac{\mu_L^2}{\sqrt{a^2+\mu_L^2}} \right\} P_\ell(\mu_L)\, d\mu_L \tag{15c}$$

where $a^2 = (1-\gamma^2)/\gamma^2$, and the Legendre polynomials are defined by $P_0(\mu_L) = 1$, $P_1(\mu_L) = \mu_L$, and the recursion relation,

$$\ell P_\ell(\mu_L) = (2\ell-1)\ \mu_L\ P_{\ell-1}(\mu_L) - (\ell-1)\ P_{\ell-2}(\mu_L)\ . \tag{16}$$

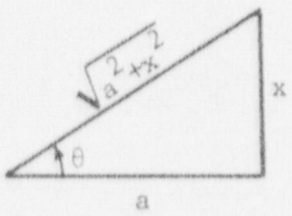
Since $P_\ell(\mu_L)$ is simply a polynomial in μ_L, it is necessary only to evaluate integrals of the form:

$$f_n(x) = \int x^n\, dx \qquad n=1,2,3,4,5,\ \ldots,\ (\ell+1) \tag{17}$$

$$g_n(x) = \int x^n \sqrt{a^2+x^2}\ dx \qquad n=0,1,2,3,4,\ \ldots,\ \ell \tag{18}$$

$$h_n(x) = \int \frac{x^n}{\sqrt{a^2+x^2}}\ dx \qquad n=2,4,5,6,7,\ \ldots,\ (\ell+2) \tag{19}$$

The integrals represented by $g_n(x)$ and $h_n(x)$ are less obvious than those represented by $f_n(x)$. In both cases, a substitution



$$\tan\theta = \frac{x}{a} \qquad \cos\theta = \frac{a}{\sqrt{a^2+x^2}}$$

$$x = a\tan\theta \qquad \sqrt{a^2+x^2} = \frac{a}{\cos\theta}$$

$$dx = a\sec^2\theta\, d\theta \qquad \sqrt{a^2+x^2} = a\sec\theta$$

of the form $x = a\tan\theta$ will prove useful. The evaluation of the $g_n(x)$ integrals will be illustrated more fully, with development of the $h_n(x)$ integrals following a similar course. As will be seen, a separate case must be made for n = odd and n = even.

For n = odd, the $g_n(x)$ integrals are evaluated as follows:

$$g_n(x) = \int x^n \sqrt{a^2+x^2}\ dx = a^{n+2} \int \tan^n\theta\, \sec^3\theta\, d\theta \tag{20}$$

$$g_n(x) = a^{n+2} \int \tan\theta \, (\sec^2\theta - 1)^m \sec^3\theta \, d\theta \,, \qquad m = \frac{n-1}{2} \quad . \tag{21}$$

Using the Binomial theorem to expand $(\sec^2\theta-1)^m$ yields:

$$\begin{aligned}(\sec^2\theta - 1)^m \sec^3\theta = \Bigg[& (\sec\theta)^{2m+3} + \left(\frac{1-k}{1}\right) (\sec\theta)^{2(m-1)+3} \\ & + \left(\frac{1-k}{1}\right)\left(\frac{2-k}{2}\right) (\sec\theta)^{2(m-2)+3} \\ & + \left(\frac{1-k}{1}\right)\left(\frac{2-k}{2}\right)\left(\frac{3-k}{3}\right) (\sec\theta)^{2(m-3)+3} \\ & + \ldots\ldots \Bigg] \,, \qquad k = m+1 \quad .\end{aligned} \tag{22}$$

Recognizing that $\tan\theta = \sin\theta/\cos\theta$ and substituting into Eq. (21) yields:

$$\begin{aligned}g_n(x) = a^{n+2} \int \Bigg[& (\cos\theta)^{-2m-4} + \left(\frac{1-k}{1}\right) (\cos\theta)^{-2(m-1)-4} \\ & + \left(\frac{1-k}{1}\right)\left(\frac{2-k}{2}\right) (\cos\theta)^{-2(m-2)-4} \\ & + \left(\frac{1-k}{1}\right)\left(\frac{2-k}{2}\right)\left(\frac{3-k}{3}\right) (\cos\theta)^{-2(m-3)-4} \\ & + \ldots\ldots \Bigg] \sin\theta \, d\theta \quad .\end{aligned} \tag{23}$$

Letting $v = \cos\theta$, $dv = -\sin\theta \, d\theta$ will allow the integral to be evaluated with ease, the result being:

$$\begin{aligned}g_n(x) = a^{n+2} \Bigg[& \left(\frac{1}{2m+3}\right) (\sec\theta)^{2m+3} + \left(\frac{1}{2(m-1)+3}\right)\left(\frac{1-k}{1}\right) (\sec\theta)^{2(m-1)+3} \\ & + \left(\frac{1}{2(m-2)+3}\right)\left(\frac{1-k}{1}\right)\left(\frac{2-k}{2}\right) (\sec\theta)^{2(m-2)+3}\end{aligned}$$

$$+ \left(\frac{1}{2(m-3)+3}\right)\left(\frac{1-k}{1}\right)\left(\frac{2-k}{2}\right)\left(\frac{3-k}{3}\right) (\sec\theta)^{2(m-3)+3}$$

$$+ \ldots\ldots\Big], \qquad n = \text{odd} \tag{24}$$

where:

$$m = (n-1)/2,$$

$$k = m+1, \text{ and}$$

$$\sec\theta = \sqrt{a^2+x^2}/a.$$

To evaluate the $g_n(x)$ integrals for n=even, one proceeds as before:

$$g_n(x) = \int x^n \sqrt{a^2+x^2}\, dx = a^{n+2} \int \tan^n\theta \sec^3\theta\, d\theta \tag{25}$$

$$g_n(x) = a^{n+2} \int (\sec^2\theta-1)^m \sec^3\theta\, d\theta, \qquad m = n/2 . \tag{26}$$

Using the Binomial theorem to expand $(\sec^2\theta-1)^m$ yields:

$$g_n(x) = a^{n+2} \int \Big[(\sec\theta)^{2m+3} + \left(\frac{1-k}{1}\right) (\sec\theta)^{2(m-1)+3}$$

$$+ \left(\frac{1-k}{1}\right)\left(\frac{2-k}{2}\right) (\sec\theta)^{2(m-2)+3}$$

$$+ \left(\frac{1-k}{1}\right)\left(\frac{2-k}{2}\right)\left(\frac{3-k}{3}\right) (\sec\theta)^{2(m-3)+3}$$

$$+ \ldots\ldots\Big] d\theta , \qquad n = \text{even} \tag{27}$$

where $m = n/2$ and $k = m+1$. This differs from the previous case insofar as one must now integrate powers of sec θ. Fortunately, this may be done analytically using a reduction formula of the form:

$$\int (\sec\theta)^j \, d\theta = \left(\frac{1}{j-1}\right) \left\{ (\sec\theta)^{j-2} \tan\theta + (j-2) \int (\sec\theta)^{j-2} \, d\theta \right\} \tag{28}$$

where

$$\int \sec\theta \, d\theta = \ln |\sec\theta + \tan\theta| = \ln(x + \sqrt{a^2+x^2}) \ . \tag{29}$$

The integral of sec θ may be easily verified by differentiating the result. The reduction formula may be proven by setting:

$u = (\sec\theta)^{n-2}$ $\qquad$ $dv = (\sec\theta)^2$

$du = (n-2) (\sec\theta)^{n-2} \tan\theta \, d\theta$ $\qquad$ $v = \tan\theta$

and integrating by parts using

$$\int u \, dv = uv - \int v \, du \ . \tag{30}$$

Applying this reduction equation repeatedly to each term in Eq. (27) will yield the analytic result for $g_n(x)$ in terms of sec θ and tan θ, where

$\sec\theta = \sqrt{a^2+x^2}/a$ $\qquad$ and $\qquad$ $\tan\theta = x/a$.

For n = odd, the $h_n(x)$ integrals may be evaluated the same as the $g_n(x)$ integrals, c.f. Eqs. (20-24), with the result that:

$$\begin{aligned} h_n(x) = a^n \Bigg[& \left(\frac{1}{2m+1}\right) (\sec\theta)^{2m+1} + \left(\frac{1}{2(m-1)+1}\right)\left(\frac{1-k}{1}\right) (\sec\theta)^{2(m-1)+1} \\ & + \left(\frac{1}{2(m-2)+1}\right)\left(\frac{1-k}{1}\right)\left(\frac{2-k}{2}\right) (\sec\theta)^{2(m-2)+1} \\ & + \left(\frac{1}{2(m-3)+1}\right)\left(\frac{1-k}{1}\right)\left(\frac{2-k}{2}\right)\left(\frac{3-k}{3}\right) (\sec\theta)^{2(m-3)+1} \\ & + \ldots\ldots \Bigg] \end{aligned} \tag{31}$$

where $m = (n-1)/2$, $k = m+1$, and $\sec\theta = \sqrt{a^2+x^2}/a$.

For n = even, the $h_n(x)$ integrals may be evaluated the same as the $g_n(x)$ integrals, c.f. Eqs. (25-27), with the result that:

$$h_n(x) = a^n \int \left[(\sec\theta)^{2m+1} + \left(\frac{1-k}{1}\right) (\sec\theta)^{2(m-1)+1} + \left(\frac{1-k}{1}\right)\left(\frac{2-k}{2}\right) (\sec\theta)^{2(m-2)+1} + \left(\frac{1-k}{1}\right)\left(\frac{2-k}{2}\right)\left(\frac{3-k}{3}\right) (\sec\theta)^{2(m-3)+1} + \ldots\ldots \right] d\theta , \qquad n = \text{even} \tag{32}$$

where $m = n/2$ and $k = m+1$. Applying the reduction equation repeatedly to each term in Eq. (32) will yield the analytic result for $h_n(x)$ in terms of sec θ and tan θ, where:

$\sec\theta = \sqrt{a^2+x^2}/a$ and $\tan\theta = x/a$.

C. Exact Treatment for Hydrogen

For elastic scattering in the center-of-mass system, $\gamma = 1/A$ where A is generally the atomic mass of the target nuclide. In the context of two body kinematics, A as used in the above equations should really be the ratio of the mass of the target nuclide to the mass of the incident neutron. The precise value of that ratio for hydrogen is somewhat less than unity (0.9991682). This would yield a value of γ just slightly greater than unity and the form of the above equations would become:

$$\int_{E^g}^{E^{g-1}} P_\ell[\mu_L(E',E,Q,A)]\ \sigma(E'\to E)\ dE =$$

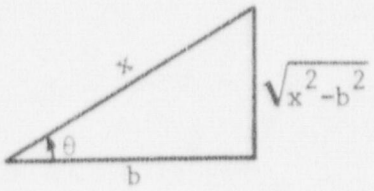
$$\frac{\gamma}{2}\,\sigma(E') \int_{\mu_L(E',E_L,Q,A)}^{\mu_L(E',E_U,Q,A)} \left\{ 2\mu_L + \sqrt{\mu_L^2 - b^2} + \frac{\mu_L^2}{\sqrt{\mu_L^2 - b^2}} \right\} P_\ell(\mu_L) \tag{33}$$

where $b^2 = \frac{\gamma^2-1}{\gamma^2} > 0$. The integrals corresponding to

$$\tilde{g}_n(x) = \int x^n \sqrt{x^2-b^2}\ dx \tag{34}$$

$$\tilde{h}_n(x) = \int \frac{x^n}{\sqrt{x^2-b^2}}\ dx \tag{35}$$

could then be evaluated analytically using substitutions of the form $x = b \sec\theta$. Using these substitutions and



$$\tan\theta = \frac{\sqrt{x^2-b^2}}{b} \qquad \cos\theta = \frac{b}{x}$$

$$x = b\sec\theta$$

$$\sqrt{x^2-b^2} = b\tan\theta \qquad dx = b\tan\theta\sec\theta\, d\theta$$

noting that $\tan^2\theta = \sec^2\theta - 1$ yields:

$$\tilde{g}_n(x) = b^{n+2}\int [(\sec\theta)^{n+3} - (\sec\theta)^{n+1}]\ d\theta \tag{36}$$

$$\tilde{h}_n(x) = b^n \int (\sec\theta)^{n+1}\ d\theta \tag{37}$$

Applying the reduction equation repeatedly to each term will yield the analytic result for $\tilde{g}_n(x)$ and $\tilde{h}_n(x)$ in terms of sec θ and tan θ, where now

$\sec\theta = x/b$ and $\tan\theta = \sqrt{x^2-b^2}/b$.

The exact treatment outlined here undoubtedly represents an unnecessary degree of accuracy. If, however, such accuracy is desired, the integral of Eq. (33) must be performed using double precision arithmetic throughout.

D. Simplified Treatment for Hydrogen

In practice, the A=1 approximation is used for hydrogen, in which case Eq. (15c) remains valid. For A=1, γ=1 and a=0, such that Eq. (15c) simplifies to:

$$\int_{E^{\ell}}^{E^{g-1}} P_{\ell}[\mu_L(E',E,Q,A)]\,\sigma(E'\to E)\,dE = \frac{\sigma(E')}{2}\int_{\sqrt{E_L/E'}}^{\sqrt{E_U/E'}} 4\mu_L P_{\ell}(\mu_L)\,d\mu_L \,. \qquad (38)$$

Since $P_{\ell}(\mu_L)$ is simply a polynomial in μ_L, it is necessary only to evaluate integrals of the form

$$f_n(x) = \int x^n\,dx = \left(\frac{1}{n+1}\right) x^{n+1} \qquad (39)$$

where for odd values of ℓ, n will take on only even values and for even values of ℓ, n will assume only odd values. In practice, this simplification for hydrogen can yield substantial savings in computing time since, for each of the several thousand initial energy points (E'), hydrogen downscatters to all lower energy groups. For heavier nuclides, the more complicated form, Eq. (15c), would have to be used, but the number of possible secondary energy groups would be much fewer.

E. Extension to Inelastic Scattering from Discrete Levels

For inelastic scattering from discrete levels, Eq. (15c) and the component integrals remain valid. In this case, however, the upper and lower limits for μ_L would depend on the excitation energy, Q, as shown in Eq. (5). Likewise, the parameter a^2 would depend on the excitation energy insofar as $a^2 = (1-\gamma^2)/\gamma^2$ where now

$$\gamma^2 = \left(\frac{1}{A^2}\right) \left[\frac{E'}{E' + \left(\frac{A+1}{A}\right) Q}\right] \tag{40}$$

Note that this will always yield $\gamma^2 < 1$ and $a^2 > 0$. With these minor changes, the analytic results remain the same as stated previously for elastic scattering in the center-of-mass system.

F. Extension to Include Anisotropic Scattering

If the Legendre coefficients, $\tilde{f}_k(E)$, of the angular scattering cross section are specified on a point-wise energy basis in the lab system such that

$$\sigma(E' \to E)\, dE = \sigma(E')\, \tilde{f}(E', \mu_L)\, 2\pi d\mu_L \quad \text{where} \tag{41}$$

$$\tilde{f}(E', \mu_L) = \sum_{k=0}^{ISCT(LAB)} \frac{2k+1}{4\pi}\, \tilde{f}_k(E')\, P_k(\mu_L) \;, \quad \text{then} \tag{42}$$

it is most expeditious to use this data directly. Substituting these equations into Eq. (7) yields:

$$\int_{E^g}^{E^{g-1}} P_\ell[\mu_L(E',E,Q,A)]\ \sigma(E'\to E)\ dE$$

$$= \frac{1}{2}\,\sigma(E') \sum_{k=0}^{ISCT(LAB)} (2k+1)\ \tilde{f}_k(E') \int_{\mu_L(E',E_L,Q,A)}^{\mu_L(E',E_U,Q,A)} P_k(\mu_L)P_\ell(\mu_L)\ d\mu_L\ . \quad (43)$$

Integrals of this form may be evaluated quickly and easily since the product, $P_k(\mu_L)P_\ell(\mu_L)$, is simply a polynomial in μ_L. Indeed, Weisbin[1] has developed a recursion relation for integrals of this form. To the extent to which the coefficients $\tilde{f}_k(E')$ reproduce experimental data, the result will be exact and analytic with no truncation error.

If, on the other hand, the Legendre coefficients, $f_k(E')$, of the angular scattering cross section are specified on a point-wise energy basis in the center of mass system such that

$$\sigma(E'\to E)\ dE = \sigma(E')\ f(E',\mu_c)\ 2\pi d\mu_c \quad \text{where} \quad (44)$$

$$f(E',\mu_c) = \sum_{k=0}^{ISCT(CM)} \frac{2k+1}{4\pi}\ f_k(E')\ P_k(\mu_c)\ , \ \text{then} \quad (45)$$

two options are available. The first option is to substitute these equations into Eq. (7) and perform the necessary integrations analytically, without converting the expansion coefficients to the L-system and without introducing any truncation error. The second option is to use a transformation technique developed by Amster[2] to convert the C-system coefficients $f_k(E')$ k=0,1,2, ..., ISCT(CM) to L-system coefficients $\tilde{f}_j(E')$ j=0,1,2, ..., ∞, truncate the L-system expansion to some order, ISCT(LAB), and perform the integrals as indicated in the preceding

paragraph. This latter approach is presently used in the MINX code.[3] Both approaches are reviewed below.

If the Legendre coefficients, $f_k(E')$, of the angular scattering cross section are known on a point-wise energy basis in the center-of-mass system, then Eq. (45) may be substituted into Eq. (44), and that in turn may be substituted into Eq. (7). The integral of interest may then be written as:

$$\int_{E^g}^{E^{g-1}} P_\ell[\mu_L(E',E\ Q,A)]\ \sigma(E'\to E)\ dE$$

$$= \frac{1}{2}\,\sigma(E') \sum_{k=0}^{ISCT(CM)} (2k+1)\ f_k(E') \int_{\mu_c(E',E_L,Q,A)}^{\mu_c(E',E_U,Q,A)} P_k(\mu_c)\ P_\ell[\mu_L(E',E,Q,A)]\ d\mu_c \qquad (46a)$$

$$= \sum_{k=0}^{ISCT(CM)} P_k(E') \int_{\mu_L(E',E_L,Q,A)}^{\mu_L(E',E_U,Q,A)} \left|\frac{d\mu_c}{d\mu_L}\right| P_k(\mu_c)\ P_\ell(\mu_L)\ d\mu_L \qquad (46b)$$

where

$$\left|\frac{d\mu_c}{d\mu_L}\right| = \gamma\left\{2\mu_L + \sqrt{a^2+\mu_L^2} + \frac{\mu_L^2}{\sqrt{a^2+\mu_L^2}}\right\}\ ,\ a^2 = \frac{1-\gamma^2}{\gamma^2} \qquad (47)$$

and

$$\mu_c = \gamma\left\{\mu_L^2 - 1 + \mu_L\sqrt{a^2+\mu_L^2}\right\}\ ,\ a^2 = \frac{1-\gamma^2}{\gamma^2} \qquad (48)$$

Without writing all of the coefficients explicitly, the point to be made

here is that the integral of interest may be evaluated analytically using the integrals $g_n(x)$ and $h_n(x)$ already defined. Since $P_k(\mu_c)$ is a polynomial in μ_c, one must consider $|d\mu_c/d\mu_L|$ times powers of μ_c. Performing the algebra and using the Binomial theorem to expand powers of μ_c yields

$$\left|\frac{d\mu_c}{d\mu_L}\right| (\mu_c)^m = \tilde{R}_m(\mu_L) + \tilde{S}_m(\mu_L)\sqrt{a^2+\mu_L^2} + \tilde{T}_m(\mu_L)\frac{1}{\sqrt{a^2+\mu_L^2}} \tag{49}$$

where $\tilde{R}_m(\mu_L)$, $\tilde{S}_m(\mu_L)$, and $\tilde{T}_m(\mu_L)$ are polynomials in μ_L. Hence, multiplying $|d\mu_c/d\mu_L|$ by the full polynomial $P_k(\mu_c)$ will only change the coefficients of these polynomials [$\tilde{R}_m(\mu_L)$, $\tilde{S}_m(\mu_L)$, and $\tilde{T}_m(\mu_L)$], as will multiplying by $P_\ell(\mu_L)$. Thus $|d\mu_c/d\mu_L|\ P_k(\mu_c)\ P_\ell(\mu_L)$ may be written as

$$\left|\frac{d\mu_c}{d\mu_L}\right| P_k(\mu_c)\ P_\ell(\mu_L) = R^{k,\ell}(\mu_L) + S^{k,\ell}(\mu_L)\sqrt{a^2+\mu_L^2} + T^{k,\ell}(\mu_L)\frac{1}{\sqrt{a^2+\mu_L^2}} \tag{50}$$

such that

$$\int_{E^g}^{E^{g-1}} P_\ell[\mu_L(E',E,Q,A)]\ \sigma(E'\to E)\ dE$$

$$= \sum_{k=0}^{ISCT(CM)} P_k(E') \int_{\mu_L(E',E_L,Q,A)}^{\mu_L(E',E_U,Q,A)} \left|\frac{d\mu_c}{d\mu_L}\right| P_k(\mu_c) P_\ell(\mu_L)\ d\mu_L \tag{51a}$$

$$= \sum_{k=0}^{ISCT(CM)} P_k(E') \left\{ \sum_n \left[r_n^{k,\ell} f_n(\mu_L) + s_n^{k,\ell} g_n(\mu_L) + t_n^{k,\ell} h_n(\mu_L) \right] \begin{matrix} \mu_L(E',E_U,Q,A) \\ \mu_L(E',E_L,Q,A) \end{matrix} \right\} \quad (51b)$$

where $R^{k,\ell}(\mu_L)$, $S^{k,\ell}(\mu_L)$, and $T^{k,\ell}(\mu_L)$ are slightly different polynomials in μ_L; $r_n^{k,\ell}$, $s_n^{k,\ell}$, and $t_n^{k,\ell}$ are the coefficients of these polynomials; and $f_n(x)$, $g_n(x)$, and $h_n(x)$ are the integrals which were previously evaluated. Note that the result is exact and analytic with no truncation error.

The second option, of course, is to convert the C-system coefficients $f_k(E')$ to L-system coefficients $\tilde{f}_j(E')$, truncate the L-system expansion to some order, ISCT(LAB), and perform the (relatively simple) integral indicated in Eq. (43).

Certainly the angular scattering cross section as defined by Eqs. (44) and (45) could also be written in the lab system as

$$\sigma(E' \to E)\, dE = \sigma(E')\, \tilde{f}(E',\mu_L)\, 2\pi\, d\mu_L \quad \text{where} \quad (52)$$

$$\tilde{f}(E',\mu_L) = \sum_{k=0}^{\infty} \frac{2k+1}{4\pi} \tilde{f}_k(E')\, P_k(\mu_L) \quad . \quad (53)$$

Since those neutrons which scatter into $d\mu_L$ about μ_L are the same neutrons that scatter into $d\mu_c$ about μ_c,

$$\tilde{f}(E',\mu_L)\, d\mu_L = f(E',\mu_c)\, d\mu_c \quad \text{and hence:} \quad (54)$$

$$\sum_{k'=0}^{\infty} \frac{2k'+1}{4\pi} \tilde{f}_{k'}(E')\, P_{k'}(\mu_L) = \sum_{k=0}^{ISCT(CM)} \frac{2k+1}{4\pi} f_k(E') P_k\left[\mu_c(\mu_L)\right] \left|\frac{d\mu_c}{d\mu_L}\right| \quad (55a)$$

$$= \gamma \sum_{k=0}^{ISCT(CM)} \frac{2k+1}{4\pi} f_k(E') P_k\left[\mu_c(\mu_L)\right] \left\{ 2\mu_L + \sqrt{a^2+\mu_L^2} + \frac{\mu_L^2}{\sqrt{a^2+\mu_L^2}} \right\} . \qquad (55b)$$

Note, however, that the L-system expansion would require an infinite number of terms, $\tilde{f}_k(E')$, to represent the quantities within the radicals on the right. In practice, the L-system expansion is truncated to some order, ISCT(LAB), thus introducing some error.

To determine the coefficients $\tilde{f}_{k'}(E')$ requires multiplying both sides of Eq. (55) by $P_{\ell'}(\mu_L)$, integrating both sides from $\mu_L = -1$ to $\mu_L = +1$ and applying orthogonality. The result is

$$\tilde{f}_{\ell'}(E') = \sum_{k=0}^{ISCT(CM)} \frac{2k+1}{2} f_k(E') \int_{\mu_L=-1}^{\mu_L=1} \left| \frac{d\mu_c}{d\mu_L} \right| P_k(\mu_c) P_{\ell'}(\mu_L) \, d\mu_L \qquad (56a)$$

$$= \sum_{k=0}^{ISCT(CM)} \frac{2k+1}{2} f_k(E') \left\{ \sum_n \left[r_n^{k,\ell'} f_n(\mu_L) + s_n^{k,\ell'} g_n(\mu_L) + t_n^{k,\ell'} h_n(\mu_L) \right]_{\mu_L=-1}^{\mu_L=1} \right\} . \qquad (56b)$$

Note that the form of the resulting integral is the same as in the previous case; hence, both methods would require an algorithm for generating the coefficients $r_n^{k,\ell}$, $s_n^{k,\ell}$, and $t_n^{k,\ell}$.

In the approximate method, the functions $f_n(\mu_L)$, $g_n(\mu_L)$, and $h_n(\mu_L)$ would have to be evaluated once and only once at $\mu_L = +1$ and $\mu_L = -1$ for each order, $\ell' = 0,1,2, \ldots,$ ISCT(LAB). Having once established each $\tilde{f}_{\ell'}(E')$, the integrals of simple polynomials, c.f. Eq. (43), would have to be evaluated for each secondary energy group for each

initial energy. These integrals should be relatively rapid to evaluate. Some truncation error will always exist but may be reduced by using an expansion of higher order, i.e., by increasing ISCT(LAB).

In the exact analytic method, the coefficients $r_n^{k,\ell}$, $s_n^{k,\ell}$, and $t_n^{k,\ell}$ could be evaluated once and stored for each (n,k,ℓ), or they could be recalculated each time the functions $f_n(\mu_L)$, $g_n(\mu_L)$, and $h_n(\mu_L)$ are evaluated. These functions would have to be evaluated once for each secondary energy group for each initial energy point, c.f. Eq. (51b). The result would be analytic and contain no truncation error.

If the Legendre coefficients, $f_k(E')$, of the angular scattering cross section are known on a point-wise energy basis in the center of mass system, then either of the two methods may be used with the trade-off in running time depending on the expansion order ISCT(LAB) required to give acceptable results.

G. Review of Another Method Based on Numerical Quadrature

In the method to be described here, it is assumed that the angular scattering cross section is known on a point-wise energy basis in the lab system such that

$$\sigma(E'\to E)\, dE = \sigma(E')\, \tilde{f}(E',\mu_L)\, 2\pi\, d\mu_L \qquad (57)$$

where the probability distribution function $\tilde{f}(E',\mu_L)$ may, for example, be specified as a Legendre expansion in the L-system. If the Legendre expansion coefficients are known only in the C-system, a conversion to the L-system is made using the procedure described earlier. Substituting Eq. (57) into Eq. (7) and noting that

$$\int_{E^g}^{E^{g-1}} P_\ell[\mu_L(E',E,Q,A)]\ \sigma(E'\rightarrow E)\ dE$$

$$= 2\pi\ \sigma(E') \int_{\mu_L(E',E_L,Q,A)}^{\mu_L(E',E_U,Q,A)} \tilde{f}(E',\mu_L)\ P_\ell(\mu_L)\ d\mu_L \qquad (58)$$

yields

$$\sigma_\ell(g'\rightarrow g) = (2\pi/\phi^{g'}) \int_{E^{g'}}^{E^{g'-1}} \phi(E')\ \sigma(E')$$

$$\left[\int_{\mu_L(E',E_L,Q,A)}^{\mu_L(E',E_U,Q,A)} \tilde{f}(E',\mu_L)\ P_\ell(\mu_L)\ d\mu_L\right] dE' \quad . \qquad (59)$$

With no loss of accuracy, this equation may be written as

$$\sigma_\ell(g'\rightarrow g) = (2\pi/\phi^{g'}) \int_{-1}^{+1} P_\ell(\mu_L)$$

$$\left[\int_{E^{g'}}^{E^{g'-1}} \phi(E')\ \sigma(E')\ \tilde{f}(E',\mu_L)\ \varepsilon(\mu_L)\ dE'\right] d\mu_L \qquad (60)$$

where

$$\varepsilon(\mu_L) = \begin{cases} 1.0 & \text{if, for } E^{g'} \le E' \le E^{g'-1}, \\ & \mu_L(E',E_L,Q,A) \le \mu_L \le \mu_L(E',E_U,Q,A) \\ 0.0 & \text{otherwise} \quad . \end{cases} \qquad (61)$$

Alternately, since μ_L is a monotonic function of E', the effect of $\varepsilon(\mu_L)$ may be incorporated in the limits of integration such that Eq. (61) may be written as:

$$\sigma_\ell(g' \to g) = (2\pi/\phi^{g'}) \int_{-1}^{+1} P_\ell(\mu_L) \left[\int_{E_{low}(\mu_L,g)}^{E_{high}(\mu_L,g)} \phi(E')\, \sigma(E')\, \tilde{f}(E',\mu_L)\, dE' \right] d\mu_L \tag{62}$$

where $E_{high}(\mu_L,g)$ and $E_{low}(\mu_L,g)$ depend on various conditions as noted in Fig. 2 with

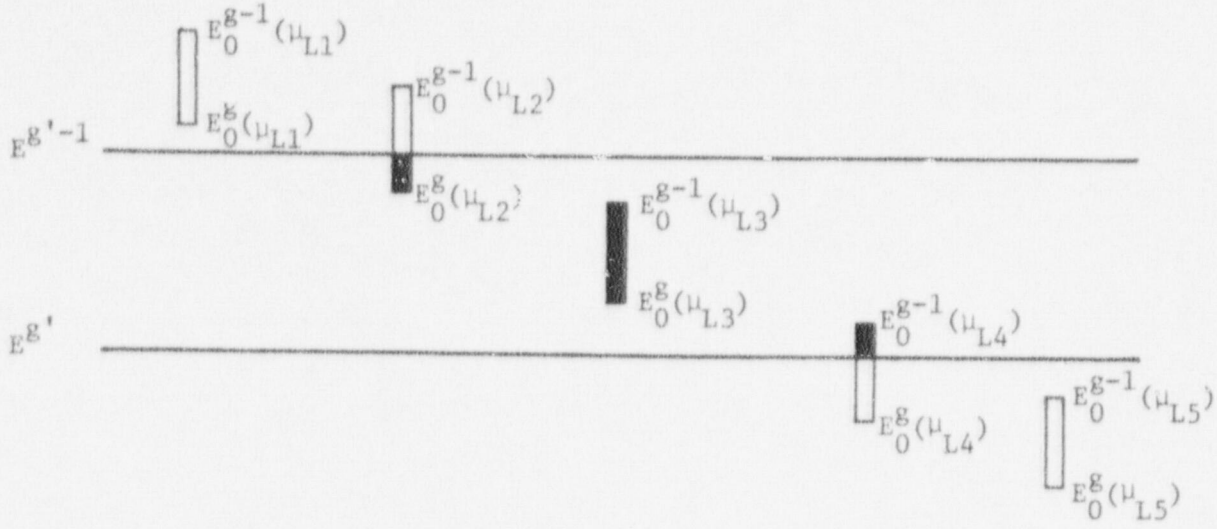
$$E_0^{g-1} = E^{g-1} \left[p(\mu_L, E^{g-1}, Q, A) \right]^2 \tag{63}$$

$$E_0^{g} = E^{g} \left[p(\mu_L, E^{g}, Q, A) \right]^2 \tag{64}$$

and

$$p(\mu_L,E,Q,A) = \begin{cases} -\left(\frac{\mu_L}{A-1}\right) + \sqrt{\left(\frac{\mu_L}{A-1}\right)^2 + \left(\frac{A+1}{A-1}\right) + \left(\frac{Q}{E}\right)\left(\frac{A}{A-1}\right)} & \text{for } A>1 \\ \left(\frac{1}{2\mu_L}\right)\left[2 + \left(\frac{Q}{E}\right)\right] & \text{for } A=1 \end{cases} \tag{65}$$

Eq. (62) is equivalent to Eqs. (59) and (60) with no loss of rigor. At this point, however, it is convenient to approximate the angular integral of Eq. (62) with a numerical quadrature of some order, N, such that



$E_{high}=0$	$E_{high}=E^{g'-1}$	$E_{high}=E_0^{g-1}$	$E_{high}=E_0^{g-1}$	$E_{high}=0$
$E_{low}=0$	$E_{low}=E_0^{g}$	$E_{low}=E_0^{g}$	$E_{low}=E^{g'}$	$E_{low}=0$

Figure 2. Location of a given primary energy group ($E^{g'-1 \rightarrow E^{g'}}$) relative to the range of possible initial energies ($E_0^{g-1 \rightarrow E_0^{g}}$) of a neutron scattering through a particular angle (μ_{Ln}) into a given secondary energy group ($E^{g-1 \rightarrow Eg}$). Also shown are the limits of integration that should be used in each case.

$$\sigma_\ell(g' \to g) \doteq (2\pi/\phi^{g'}) \sum_{n=1}^{N} w_n P_\ell(\mu_{Ln})$$

$$\int_{E_{low}(\mu_{Ln},g)}^{E_{high}(\mu_{Ln},g)} \phi(E')\, \sigma(E')\, \tilde{f}(E',\mu_{Ln})\, dE' \qquad (66)$$

As a practical matter, values of N=8 up to N=16 are commonly used. To the extent that the angular scattering distribution function, $\tilde{f}(E',\mu_L)$, is independent of E' over certain broad ranges, it may be taken outside the energy integral. The evaluation of the group-to-group Legendre transfer coefficients is then reduced to evaluating the integral of $\phi(E')\sigma(E')$ over certain broad ranges in which $\sigma(E')$ is specified by one of the five ENDF interpolation formulas (flat, linear-linear, log-linear, linear-log, or log-log) and $\phi(E')$ may be $1/E'$ or some other assumed form. Such integrals can be performed analytically with great speed.

The approach described above, based on Eq. (66), has been successfully used in an experimental version of the XLACS code[4,5,6] The results have generally been quite good except in the case of hydrogen (in which case XLACS now reverts to a more direct numerical approach). The method does, however, have some difficulties as described below.

Given a sufficiently small secondary energy group, the above method yields at most N group-to-group transfers for which $\sigma_\ell(g' \to g)$ may be non-zero. (That is: Let $\Delta E^g_{0n} = E^{g-1}_{0n} - E^g_{0n}$ correspond to angle μ_{Ln}. As ΔE^g becomes small, ΔE^g_{0n} becomes small. If each ΔE^g_{0n} is sufficiently small, each ΔE^g_{0n} will lie wholly within a single primary energy group

$\Delta E^{g'}$. If each ΔE^{g}_{0n} lies within a separate primary energy group, there will be (at most) N group-to-group transfers for which $\sigma_\ell(g' \to g)$ may be non-zero.) This problem is most noticeable in the case of light nuclides. With hydrogen, for example, the present method yields $\sigma_0(g' \to g) = 0$ for many group-to-group transfers when, in fact, neutrons can scatter into a particular group from all higher energy groups and $\sigma_0(g' \to g)$ should be non-zero whenever $g' \leq g$. In addition, the numerical values of the non-zero transfer coefficients may be in error, as noted below.

For the purpose of explaining some aspects of the method, it is convenient to combine the numerical quadrature of Eq. (66) and the notation used in Eq. (60). Thus Eq. (66) may be re-written as

$$\sigma_\ell(g' \to g) \doteq (2\pi/\phi^{g'}) \sum_{n=1}^{N} w_n P_\ell(\mu_{Ln}) \int_{E^{g'}}^{E^{g'-1}} \phi(E') \sigma(E') \tilde{f}(E', \mu_{Ln}) \varepsilon(\mu_{Ln}) dE' \qquad (67)$$

where $\varepsilon(\mu_{Ln})$ is defined by Eq. (61). If $\tilde{f}(E', \mu_L)$ is a polynomial in μ_L and N represents a sufficiently large Gaussian quadrature, then Eq. (67) will yield on exact value for $\sigma_\ell(g' \to g)$ if and only if $\varepsilon(\mu_{Ln}) = 1.0$ for each angle μ_{Ln} When, for a given group-to-group transfer, $\varepsilon(\mu_{Ln}) = 0.0$ for any of the N angles (μ_{Ln}), the numerical value of $\sigma_\ell(g' \to g)$ represents an approximation which should be examined. If the group structure is sufficiently fine, there will be precisely N group-to-group transfers for which $\sigma_\ell(g' \to g)$ will be non-zero and each of these will have only one (as opposed to all N) angles μ_{Ln} for which $\varepsilon(\mu_{Ln}) = 1.0$ and the numerical values of $\sigma_\ell(g' \to g)$ should certainly be

held suspect.* Use of the approximation with a broader group structure will improve the accuracy of the results since each group-to-group transfer will then encompass more angles for which $\varepsilon(\mu_{Ln})$ will be non-zero. For a physically possible group-to-group transfer within a given group structure, examination of Eq. (5) and Eq. (61) reveals that the number of angles for which $\varepsilon(\mu_{Ln}) = 1.0$ increases as A increases. Thus, the numerical values of $\sigma_\ell(g' \to g)$ obtained for heavy nuclides are better than those obtained for light nuclides. Numerical experiments do, in fact, indicate the approximation to be quite good for heavy nuclides and adequate for all nuclides but hydrogen. In all cases, the accuracy of the approximation may be increased by increasing N.

While the above method may have some difficulties calculating the individual group-to-group scattering cross sections, $\sigma_\ell(g' \to g)$, it is worthwhile to note that the total scattering cross section for a given group

$$\sigma_\ell(g') = \sum_{g=1}^{G} \sigma_\ell(g' \to g) \tag{68}$$

---

*While the quadrature method (of some fixed order, N) does indeed fail to yield accurate values of $\sigma_\ell(g' \to g)$ when the group structure becomes sufficiently fine, the utility of even an exact method must be considered in order to retain perspective. When the group structure is sufficiently fine, $\sigma(g' \to g, \mu_L)$ will physically be non-zero over only a very narrow range of μ_L and an adequate representation of the angular scattering distribution using a Legendre expansion may require many terms, $\sigma_\ell(g' \to g)$. Present day computers place a practical limit on the number of such terms that can be carried in a given transport calculation.

will remain correct. Taking the summation on g inside Eq. (67) yields

$$\sigma_\ell(g') = (2\pi/\phi^{g'}) \sum_{n=1}^{N} w_n P_\ell(\mu_{Ln})$$

$$\int_{E^{g'}}^{E^{g'-1}} \phi(E') \sigma(E') \tilde{f}(E',\mu_{Ln}) \left[\sum_{g=1}^{G} \varepsilon(\mu_{Ln}) \right] dE' \qquad (69)$$

If $\tilde{f}(E',\mu_L)$ is a polynomial in μ_L and N represents a sufficiently large Gaussian quadrature, then Eq. (69) will yield on exact value for $\sigma_\ell(g')$ if and only if

$$\sum_{g=1}^{G} \varepsilon(\mu_{Ln}) = 1.0 \qquad (70)$$

for each angle μ_{Ln}. A neutron initially at energy E' scattering through a fixed angle μ_{Lj} loses a specific amount of energy and lands up in one and only one energy group, g*. Thus, $\varepsilon(\mu_{Lj}) = 1.0$ for that energy group and 0.0 for all others. Thus Eq. (70) is satisfied for that particular angle μ_{Lj}. The same argument may, of course, be made for each of the N angles, thus satisfying the necessary condition.

H. FORTRAN Routine for Isotropic, Elastic Scattering in the C-System

Many scattering processes can be hypothesized on theoretical grounds to be isotropic in the center-of-mass system. Such is usually the case whenever a compound nucleus is formed. Hence, the exact analytic treatment of such scattering as described in Section B is of special interest. A FORTRAN IV function called PINT has been written

to evaluate the integral

$$\int_{\mu_c(E',E_L,Q=0,A)}^{\mu_c(E',E_U,Q=0,A)} P_\ell[\mu_L(E',E(\mu_c),Q=0,A)]\, d\mu_c \qquad (71)$$

which is required in Eq. (15a) during the evaluation of Eq. (7).

PINT(EINIT,ESECUP,ESECLO,AA,LL) is a REAL*4 FUNCTION, the same as SIN(X) or COS(X). It has four REAL*4 arguments and one INTEGER*4 argument. The value of the function represents

$$\text{PINT} \equiv \int_{\mu_c^{\text{LOWER}}}^{\mu_c^{\text{UPPER}}} P_{LL}(\mu_L)\, d\mu_c \qquad (72)$$

where μ_L and μ_c are the direction cosines in the lab and center of mass systems, LL is the order of the desired Legendre polynomial (ℓ) and AA is the mass number of the target nuclide. EINIT is the initial energy of the neutron in the lab system. ESECUP and ESECLO are the upper and lower energy limits of the secondary energy group under consideration. From these, the appropriate limits of integration are determined subject to the constraint that $((AA-1)/(AA+1))^2$ EINIT $\leq E^{sec} \leq$ EINIT. The result is calculated analytically for $0 \leq LL \leq 20$. The routine is written so as to take advantage of the simplified treatment for hydrogen (c.f., Section D).

The CPU time required per call increases roughly as (LL/2) and is a factor of 10 less for A=1 than for A>1. The additional CPU time required to do the angular integration using PINT appears to be acceptable when compared with the time required to do the other necessary calculations in a sophisticated cross section production code. The time

required for such calculations varies strongly with the group structure and the number of groups to which downscatter can occur.

The PINT routine has been implemented in an experimental cross-section code called ROLAIDS.[7] Using 21,000 initial energy points, both a 218 group and a 16 group cross-section set were produced for each of six nuclides including hydrogen, oxygen, and uranium. P_0, P_1, and P_2 transfer matrices were produced in each case. Production of the 218 group cross sections required 5.1 minutes on the IBM-360/95(OS) while the 16 group cross-section set required only 1.4 minutes.[8]

ACKNOWLEDGMENTS

Helpful and stimulating discussions with R. M. Westfall and N. M. Greene are gratefully acknowledged. The author would also like to thank Becky Eddlemon for typing this report.

This work was performed for the U. S. Nuclear Regulatory Commission under Interagency Agreement 40-494-75.

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APPENDIX A

```
      FUNCTION PINT(EINIT,ESECUP,ESECLO,AA,LL)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 PINT,EINIT,ESECUP,ESECLO,AA
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      PINT = 0.0
      IF (ESECLO.GT.EINIT)  RETURN
      ALPHA = (AA-1.0)/(AA+1.0)
      ALPHA = ALPHA*ALPHA
      AELOW = ALPHA*EINIT
      IF (ESECUP.LT.AELOW)  RETURN
      ESECU = ESECUP
      ESECL = ESECLO
      IF (ESECUP.GT.EINIT)  ESECU=EINIT
      IF (ESECLO.LT.AELOW)  ESECL=AELOW
      ULUP = SQRT(ESECU/EINIT)
      IF (AA.LT.1.01)  GO TO 2
      ULUP = (AA+1.0)*ULUP-(AA-1.0)/ULUP
      ULUP = ULUP/2.0
    2 ULLO = SQRT(ESECL/EINIT)
      IF (AA.LT.1.01)  GO TO 3
      ULLO = (AA+1.0)*ULLO-(AA-1.0)/ULLO
      ULLO = ULLO/2.0
    3 AAAA = AA*AA-1.0
      A = SQRT(AAAA)
      CALL PGEN (LL)
      LLTEST = INT(0.1+2.0*FLOAT(LL/2))
      IF (LLTEST.EQ.LL)  PINT=(PINTE(LL,A,ULUP)-PINTE(LL,A,ULLO))/AA
      IF (LLTEST.LT.LL)  PINT=(PINTO(LL,A,ULUP)-PINTO(LL,A,ULLO))/AA
      RETURN
      END
```

```
      SUBROUTINE PGEN (LL)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ANTPLU/AISEC(23),BISEC(21),CIU(22),QA(21),QB(21)
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      LLP1 = LL+1
      DO 2 I=1,LLP1
      QA(I) = 0.0
    2 QB(I) = 0.0
      QB(1) = 1.0
      IF (LL.EQ.0)  RETURN
      QB(1) = 0.0
      QA(1) = 1.0
      QB(2) = 1.0
      IF (LL.EQ.1)  RETURN
      DO 6 L=2,LL
      IUP = L-1
      DO 4 I=1,IUP
    4 QA(I) = FLOAT(1-L)*QA(I)/FLOAT(L)
      IUP = L+1
      DO 5 I=2,IUP
      J = I-1
    5 QA(I) = QA(I)+QB(J)*FLOAT(L+L-1)/FLOAT(L)
      DO 6 I=1,IUP
      DUM = QA(I)
      QA(I) = QB(I)
    6 QB(I) = DUM
      RETURN
      END
```

```
      FUNCTION PINTE(LL,A,UL)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ANTPLU/AISEC(23),BISEC(21),CIU(22),QA(21),QB(21)
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      LLP1 = LL+1
      LLP2 = LL+2
      LLP3 = LL+3
      CALL FEOINT (LLP2,UL)
      IF (A.GT.0.141775)  CALL GHEINT (LLP3,A,UL)
      PINTE = 0.0
      DO 2 LQB=1,LLP1,2
      N = LQB-1
    2 PINTE = PINTE+QB(LQB)*FUNE(N,A,UL)
      RETURN
      END
```

```
      FUNCTION PINTO(LL,A,UL)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ANTPLU/AISEC(23),BISEC(21),CIU(22),QA(21),QB(21)
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      LLP1 = LL+1
      LLP2 = LL+2
      CALL FEOINT (LLP2,UL)
      IF (A.GT.0.141775)  CALL GHOINT (LLP2,A,UL)
      PINTO = 0.0
      DO 2 LQB=2,LLP1,2
      N = LQB-1
    2 PINTO = PINTO+QB(LQB)*FUNO(N,A,UL)
      RETURN
      END
```

```
      FUNCTION FUNE(N,A,UL)
      IMPLICIT REAL*8 (A-H,O-Z)
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      NFEO = N+1
      IF (A.GT.0.141775)  GO TO 2
      FUNE = 4.0*FEO(NFEO,UL)
      RETURN
    2 NH = N+2
      FUNE = GE(N,A,UL)+HE(NH,A,UL)
      FUNE = (2.0*FEO(NFEO,UL)+FUNE)
      RETURN
      END

      FUNCTION FUNO(N,A,UL)
      IMPLICIT REAL*8 (A-H,O-Z)
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      NFEO = N+1
      IF (A.GT.0.141775)  GO TO 2
      FUNO = 4.0*FEO(NFEO,UL)
      RETURN
    2 NH = N+2
      FUNO = GO(N,A,UL)+HO(NH,A,UL)
      FUNO = (2.0*FEO(NFEO,UL)+FUNO)
      RETURN
      END
      FUNCTION FEO(N,UL)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ANTPLU/AISEC(23),BISEC(21),CIU(22),QA(21),QB(21)
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      NP1 = N+1
      FEO = CIU(NP1)/FLOAT(NP1)
      RETURN
      END

      SUBROUTINE FEOINT (NP1,X)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ANTPLU/AISEC(23),BISEC(21),CIU(22),QA(21),QB(21)
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      CIU(1) = X
      DO 2 I=2,NP1
      J = I-1
    2 CIU(I) = X*CIU(J)
      RETURN
      END
```

14071

```
      FUNCTION GE(N,A,UL)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ANTPLU/AISEC(23),BISEC(21),CIU(22),QA(21),QB(21)
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      NP3 = N+3
      GE = AISEC(NP3)
      IF (N.EQ.0) GO TO 6
      M = N/2
      K = M+1
      TERM = 1.0
      ITERM = 0
    2 ITERM = ITERM+1
      I = 2*(M-ITERM)+3
      TERM = TERM*FLOAT(ITERM-K)/FLOAT(ITERM)
      GE = GE+TERM*AISEC(I)
      IF (I.NE.3) GO TO 2
    6 DO 5 I=2,NP3
    5 GE = GE*A
      RETURN
      END



      FUNCTION HE(N,A,UL)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ANTPLU/AISEC(23),BISEC(21),CIU(22),QA(21),QB(21)
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      NP1 = N+1
      HE = AISEC(NP1)
      IF (N.EQ.0) RETURN
      M = N/2
      K = M+1
      TERM = 1.0
      ITERM = 0
    2 ITERM = ITERM+1
      I = 2*(M-ITERM)+1
      TERM = TERM*FLOAT(ITERM-K)/FLOAT(ITERM)
      HE = HE+TERM*AISEC(I)
      IF (I.NE.1) GO TO 2
      DO 5 I=1,N
    5 HE = HE*A
      RETURN
      END
```

```
      SUBROUTINE GHEINT (NP3,A,X)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ANTPLU/AISEC(23),BISEC(21),CIU(22),QA(21),QB(21)
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      DO 1 I=1,NP3
    1 AISEC(I) = 0.0
      R = SQRT(A*A+X*X)
      SSEC = R/A
      TTAN = X/A
      AISEC(1) = ALOG(SSEC+TTAN)
      TERM = 1.0/SSEC
      TMULT = SSEC*SSEC
      DO 2 I=3,NP3,2
      J = I-2
      AISEC(I) = FLOAT(J)*AISEC(J)
      TERM = TMULT*TERM
      DUM = TTAN*TERM+AISEC(I)
    2 AISEC(I) = DUM/FLOAT(I-1)
      RETURN
      END
```

```
      FUNCTION GO(N,A,UL)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ANTPLU/AISEC(23),BISEC(21),CIU(22),QA(21),QB(21)
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      NP2 = N+2
      GO = BISEC(NP2)/FLOAT(NP2)
      IF (N.EQ.1)  GO TO 6
        = (N-1)/2
        = M+1
      TERM = 1.0
      ITERM = 0
    2 ITERM = ITERM+1
      I = 2*(M-ITERM)+3
      TERM = TERM*FLOAT(ITERM-K)/FLOAT(ITERM)
      GO = GO+TERM*BISEC(I)/FLOAT(I)
      IF (I.NE.3)  GO TO 2
    6 DO 5 I=1,NP2
    5 GO = GO*A
      RETURN
      END



      FUNCTION HO(N,A,UL)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ANTPLU/AISEC(23),BISEC(21),CIU(22),QA(21),QB(21)
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      HO = BISEC(N)/FLOAT(N)
      IF (N.EQ.1)  GO TO 6
      M = (N-1)/2
      K = M+1
      TERM = 1.0
      ITERM = 0
    2 ITERM = ITERM+1
      I = 2*(M-ITERM)+1
      TERM = TERM*FLOAT(ITERM-K)/FLOAT(ITERM)
      HO = HO+TERM*BISEC(I)/FLOAT(I)
      IF (I.NE.1)  GO TO 2
    6 DO 5 I=1,N
    5 HO = HO*A
      RETURN
      END
```

```
      SUBROUTINE GHOINT (NP2,A,X)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/ANTPLU/AISEC(23),BISEC(21),CIU(22),QA(21),QB(21)
      FLOAT(N) = DFLOAT(N)
      INT(X) = IDINT(X)
      SQRT(X) = DSQRT(X)
      ALOG(X) = DLOG(X)
      DO 1 I=1,NP2
    1 BISEC(I) = 0.0
      R = SQRT(A*A+X*X)
      SSEC = R/A
      DUM = SSEC*SSEC
      BISEC(1) = SSEC
      DO 2 I=3,NP2,2
      J = I-2
    2 BISEC(I) = DUM*BISEC(J)
      RETURN
      END
```

NRC FORM 335 (7-77) U.S. NUCLEAR REGULATORY COMMISSION

BIBLIOGRAPHIC DATA SHEET

1. REPORT NUMBER (Assigned by DDC): NUREG/CR-0295

4. TITLE AND SUBTITLE (Add Volume No., if appropriate)

A Method of Generating Multigroup Transfer Matrices Using an Analytic Angular Integration Free of Truncation Error.

2. (Leave blank)

3. RECIPIENT'S ACCESSION NO.

7. AUTHOR(S)

J. A. Bucholz

5. DATE REPORT COMPLETED: MONTH July YEAR 1978

9. PERFORMING ORGANIZATION NAME AND MAILING ADDRESS (Include Zip Code)

Oak Ridge National Laboratory
Nuclear Engineering Applications
Oak Ridge, TN 37830

DATE REPORT ISSUED: MONTH Sept. YEAR 1978

6. (Leave blank)

8. (Leave blank)

12. SPONSORING ORGANIZATION NAME AND MAILING ADDRESS (Include Zip Code)

Office of Nuclear Material Safety and Safeguards
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555

10. PROJECT/TASK/WORK UNIT NO.

11. CONTRACT NO.

FIN No. B0009

13. TYPE OF REPORT

PERIOD COVERED (Inclusive dates)

15. SUPPLEMENTARY NOTES

14. (Leave blank)

16. ABSTRACT (200 words or less)

The evaluation of generalized multigroup transfer matrices for transport calculations required a double integration extending over the primary and secondary energy groups where, for a given initial energy, the integration over the secondary energy group may be replaced by an integral over the possible scattering angles. The XLACS cross-section processing code presently used in the AMPX system treats this angular integral in an approximate manner. The more recent MINX cross-section processing code treats this angular integral analytically but can admit some small truncation error. These treatments are reviewed along with their weaknesses. In the present work, analytic expressions for these angular integrals are derived which are free of truncation error. Straightforward extensions to include inelastic and/or anisotropic scattering are included. FORTRAN routines are provided for nuclides having isotropic elastic scattering in the center-of-mass system.

17. KEY WORDS AND DOCUMENT ANALYSIS

17a. DESCRIPTORS

17b. IDENTIFIERS/OPEN-ENDED TERMS

18. AVAILABILITY STATEMENT

Unlimited

19. SECURITY CLASS (This report)

21. NO. OF PAGES

20. SECURITY CLASS (This page)

22. PRICE $

NRC FORM 335 (7-77)

1076